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NBSIR 79-1777

A Compendium of Gas Phase Basicity and Proton Affinity Measurements

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April 1979

Issued July 1979

This work was supported in part by the:

National Heart, Lung, and Blood Institute
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SEP 20 1979

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U.S. DEPARTMENT OF COMMERCE, Juanita M. Kreps, *Secretary*
Jordan J. Baruch, *Assistant Secretary for Science and Technology*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

FOREWORD

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards, but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated numerical data. These tables are published in the Journal of Physical and Chemical Reference Data, the various publication series of the National Bureau of Standards, and through other appropriate channels.

The present report consists of tables of data on gas phase basicity and proton affinity of molecules. It represents a contribution from the Ion Energetics Data Center, prepared in collaboration with staff of NHLBI, NIH and Fein-Marquart Associates. Support for the preparation of these tables has been provided by the National Heart, Lung, and Blood Institute and the Office of Standard Reference Data.

David R. Lide, Jr.
Chief, Office of Standard
Reference Data

ABSTRACT

Numerical values of experimental measurements, calculations and estimations of gas phase basicities and proton affinites are presented. Where appropriate they are recalculated to common values for the proton affinity of ammonia and the heat of formation of the proton. The annotated information is ordered by molecular formula following the Hill System. Indices are given to permit location of information by numerical value of the measurement(s), the compound formula, name and synonym, and CAS Registry Number. The literature coverage is essentially complete through 1977.

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1. INTRODUCTION

1.1 The Data Base

The present compendium tabulates all experimental measurements of gas phase basicities and measurements or derived values of proton affinities available up to the end of 1977. This compilation was carried out for the NIH-EPA CIS project which is developing a comprehensive chemical data base for the use of workers concerned with research on environmental and health problems and related areas. The numerical information presented here is also accessible and searchable by computer through the NIH/EPA Chemical Information System (CIS)(1).

1.2 Definitions and units

The gas phase basicity (GB) of a molecule (M) is defined as the negative of the Gibbs free energy change for the process

$$M + H^+ \rightarrow MH^+$$

and the proton affinity (PA) is defined as the negative of the enthalpy change for the same process.

$$PA(M) = \Delta H_f(M) + \Delta H_f(H^+) - \Delta H_f(MH^+)$$

For completeness, the temperature has to be specified. It is generally desired to evaluate the quantity at room temperature. Occasionally experiments are carried out at high temperatures (e.g. 600 K or at undefined temperatures (threshold measurements)), and for these it is necessary to apply the appropriate thermochemical corrections or threshold interpretations.

From the relation $\Delta G = \Delta H - T\Delta S$ the proton affinity can be determined from the gas phase basicity if the temperature and the entropy change of the process are known or can be estimated.

The unit in most widespread use is the kcal/mol and this unit is adopted throughout. It is related to the recommended SI unit by 1 kcal = 4.1840 kJ, exactly.

1.3 Standard states, conventions, and reference values

The process

$$M + H^+ \rightarrow MH^+$$

makes no reference to an electron and no difficulties arise if the heats and free energies of formation of all species are defined with the same ionic standard state. Unfortunately this has not always been the case.

Historically, the community determining ion heats of formation by threshold measurements have assumed the convention that the electron is at rest (as it surely is at threshold) and that it remains at rest even when deducing finite (or room) temperature heats of formation of the ions. This convention is also adopted in the two major compilations of gaseous ion thermochemistry (2,3).

The two principal compilations of neutral thermochemistry (4,5) assign to the electron a classical heat capacity, Cp, of 5/2 R. Thus at room temperature the heats of formation of all ions will be larger than those in, for example Energetics of Gaseous Ions (GIE) (3) by an amount equal to

$$\int_0^{298.15} C_p dT = \frac{5}{2} RT = 1.481 \text{ kcal/mol}$$

Calculations of proton affinities using room temperature ion heats of formation from threshold measurements as compiled and evaluated in Energetics of Gaseous Ions (3) and the proton heat of formation as given in the NBS Tech Note 270 series (4) or the JANAF tables (5) will be in error (too large) by this amount. Wherever the original reference quoted proton affinity values were in error for this reason, we have made the appropriate correction. When the heat of formation of the ion M^+, is defined according to the GIE convention, the value for the heat of formation of the proton at 298.15 K is 365.7 kcal/mol. This subject is discussed in detail in a recent review article (6).

A major part of the measurement base consists of relative measurements which can be put on an absolute basis by relating to a small number of absolute values. Unfortunately, the magnitude of some of the absolute values is still in doubt. For instance, many of the extensive scales of proton affinity ladders which have been published (7,8) have ultimately been related to the heat of formation of $t\text{-}C_4H_9^+$ as a primary standard, although the values are usually cited relative to the proton affinity of a secondary standard, ammonia. At the time the present compilation was carried out, the latter value was considered to be established at 202.3 kcal/mol (6), and it is this number which is used as the standard for the values cited here. More recent redeterminations of the heat of formation (9,10) and ionization potential (11) of the t-butyl radical, as well as additional information on the entropy change associated with the deprotonation of $t\text{-}C_4H_9^+$ (12), have resulted in a revised estimate that the proton affinity of ammonia is

greater than or equal to 207.0 kcal/mol (6). Thus, the absolute values of proton affinities given here based on relative ΔG measurements and expressed "relative to ammonia" are, according to the most recent information, too low by at least 5 kcal/mol. In this and other cases we have indicated the species to which the relative measurement is referred, so that readjustment can be made as additional information becomes available.

1.4 References

1. S. R. Heller, G. W. A. Milne, and R. J. Feldmann, "A Computer Based Chemical Information System," Science 195, 253 (1977).
2. J. L. Franklin, J. G. Dillard, H. M. Rosenstock, J. T. Herron, K. Draxl, and F. H. Field, "Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions," NSRDS-NBS-26, June 1969.
3. H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron, "Energetics of Gaseous Ions," J. Phys. Chem. Ref. Data 6 Supplement 1 (1977).
4. D. D. Wagman, et al, "Selected Values of Chemical Thermodynamics Properties," NBS Technical Note 270-3, January 1968, and subsequent Tech Notes in this series.
5. D. R. Stull and H. Prophet, "JANAF Thermochemical Tables," Second Edition, NSRDS-NBS-37, June 1971 and supplements published in J. Phys. Chem. Ref. Data.
6. S. Lias, "Thermochemistry of Polyatomic Cations," in "Kinetics of Ion-Molecule Reactions," (P. Ausloos, ed.) Plenum Press, New York, pg. 233.
7. J. F. Wolf, R. H. Staley, I. Koppel, M. Taagepera, R.

T. McIver, Jr., J. L. Beauchamp, and R. W. Taft, "Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements," J. Am. Chem. Soc. 99, 5417 (1977).

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10. M. Rossi and D. M. Golden, J. Am. Chem. Soc. submitted for publication.
11. F. A. Houle and J. L. Beauchamp, "Photoelectron Spectroscopy of Methyl, Ethyl, Isopropyl, and Tert-Butyl Radicals. Implications for the Thermochemistry and Structures of the Radicals and their Corresponding Carbonium Ions," J. Am. Chem. Soc., in press.
12. P. Ausloos and S. G. Lias "Entropy Changes for the Protonation of Alkenes," J. Am. Chem. Soc. 100, 1953 (1978).

2. THE MEASUREMENT TECHNIQUES

2.1 Absolute measurements

These are generally based on measurement of the heat of formation of a proton-containing species by a threshold

process, such as

$$H_2O_2 + h\nu \rightarrow HO_2^+ + H + e$$

From the threshold energy of this process and the heats of formation of the neutral atomic and molecular species one can deduce heat of formation of $HO2^+$, and by further straightforward calculation the proton affinity of molecular oxygen. In actual practice considerable care has to be exercised to establish the temperature to which the heat of formation refers. Threshold measurements leading to more or less accurate absolute values have been carried out by photoionization (PI), monoenergetic election impact (EM) and conventional electron impact (EI) techniques. The accuracy of these techniques has been comprehensively discussed in a recent review article (1).

2.2 Equilibrium measurements

From a determination of the proton transfer equilibrium constant for

$$AH^+ + B \rightleftarrows A + BH^+$$

one can determine the Gibbs free energy change of the reaction. This gives the basicity difference between the two compounds. In order to determine the proton affinity difference it is necessary to determine the entropy change of the reaction. The most direct and unambiguous method is to measure the equilibrium constant as a function of temperature, which yields the proton affinity directly from the Van't Hoff relation

$$\frac{d\ln K_{eq}}{d(1/T)} = \frac{-\Delta H}{R}$$

So far for proton transfer equilibria this has only been performed in a few instances, with varying degrees of success (2). Most estimates of the relative proton affinity are based on assumptions about the entropy change. These range from consideration of symmetry changes in the reaction, to reasoning by analogy, to the assumption that the entropy change is zero. The method or the assumptions made for obtaining a value for ΔS are indicated in this compendium for each determination.

Equilibrium constant measurements are carried out in three quite distinct experimental systems operating at rather different pressures. These are the high pressure ion source coupled to a mass spectrometer (MS), the flowing afterglow tube (FAG) whose equilibrium ion composition is sampled by a quadrupole mass spectrometer, and ions trapped for finite time in a cyclotron field (ICR) with subsequent ejection and analysis by rf absorption. These techniques have been discussed in detail in a number of reviews (2-6).

2.3 Bracketing measurements

The same techniques described immediately above can be used to examine the occurrence or non-occurrence of a proton transfer reaction, and applying the criterion that occurrence implies a negative free energy change and non-occurrence implies a positive free energy change. Accepting these assumptions, one could in principle bracket the range which the gas phase basicity of a molecule lies (7). Using different reagent ions many authors have reported such relative basicities as relative "proton affinities". Results

obtained from this approach should be used only with great caution; it is now well known that many endoergic reactions may occur with a rate constant high enough that they can easily be observed under the experimental conditions described above (3). Furthermore, many proton transfer reactions which are clearly exothermic are not observed to occur if more favorable reaction channels exist (8).

2.4 Calculations and estimates

In principle, proton affinities or ion heats of formation can be calculated quantum mechanically. We include here only the very high quality calculations carried out on $H3^+$ (see Tables). Another type of calculation deals with the evaluation of the lattice energy of an ionic crystal (CLE) (9). For an ammonium halide, for example, this gives the energy of the crystal relative to the gas phase ammonium and halide ions. These can then be related to gas phase neutral species via a Born-Haber cycle, and will yield the proton affinity of NH3(gas). Lastly, there are a number of empirical correlations of proton affinities with other physical parameters such as core ionization potentials (10).

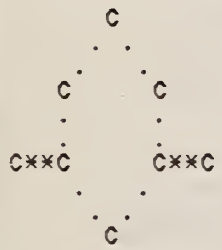
2.5 References

1. H. M. Rosenstock, "The Measurement of Ionization and Appearance Potentials," Int. J. Mass Spectrom. Ion Phys. 20, 139 (1976).
2. S. G. Lias, "Thermodynamic Information from Ion-Molecule Equilibrium Constant Determinations," in "Ion Cyclotron Resonance Spectrometry" (H. Hartmann and K.-P. Wanczek, eds.), Springer- Verlag, Berlin (1978).

3. S. Lias, "Thermochemistry of Polyatomic Cations," in "Kinetics of Ion Molecule Reactions," (P. Ausloos, Ed.), Plenum Press, New York (1979), pg. 233.
4. P. Kebarle, "Ion Thermochemistry and Solvation from Gas Phase Ion Equilibria," Ann. Rev. Phys. Chem. 28, 445 (1977).
5. D. H. Aue and M. T. Bowers, "Stabilities of Positive Ions from Equilibrium Gas Phase Basicity Measurements," in "Gas Phase Ion Chemistry," (M. T. Bowers, ed.), Academic Press, New York (1979).
6. D. K. Bohme, "The Kinetics and Energetics of Proton Transfer," in "Interactions between Ions and Molecules," (P. Ausloos, ed.), Plenum Press, New York (1975).
7. J. Long and B. Munson, "Proton Affinities of some Oxygenated Compounds," J. Am. Chem. Soc. 95, 2427 (1973).
8. P. Ausloos and S. G. Lias, "Proton Affinity of Dichlorocarbene," J. Am. Chem. Soc. 100, 4594 (1978).
9. J. Sherman, "Crystal Energies of Ionic Compounds and Thermochemical Applications," Chem. Rev. 11, 93 (1932).
10. J. A. Jen and T. D. Thomas, "Core Ionization Potentials in Dimethyl Ether and Methylamine," J. Electron Spectrosc. 4, 43 (1974).

3. ORGANIZATION OF THE INFORMATION

3.1 A typical measurement entry is shown below:

C8H10	CAS REGN : 108-38-3
	
Benzene, 1,3-dimethyl- (9CI) m-Xylene (8CI)	
GB (exp) : 182+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 189.7+/-3 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).	
Method used : MS Equilibrium relative to CH3SH and (CH3)2O Entropy change assumed zero	
GB (exp) : 187.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 298 K
Devlin, J. L., III, Wolf, J. F., Taft, R. W., and Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to C6H6(Benzene)	

The entry gives successively the following information:

a) The empirical formula in Hill System order.
b) The Chemical Abstracts Service (CAS) Registry Number.
c) The structural formula (see discussion below).
d) The Chemical Abstracts Service (CAS) Name, as given in the 8th Collective Index (8CI) and the 9th Collective Index (9CI). If it is the same in both it is denoted with (8CI9CI).
e) The gas phase basicity, GB, in kcal/mol.
f) The proton affinity, PA, in kcal/mol.
g) The temperature at which the measurement was carried out.
h) The literature citation.
i) The method used (see discussion below).
j) Additional comments on the nature of the measurement.

Where there are several measurements on the same species, the numerical value, literature reference, method and associated comments are listed successively.

The structural diagrams used in this publication have been generated from connection tables by the Structure and Nomenclature Search System (SANSS), one of the components of the CIS. The following symbols have been used to represent the different types of chemical bonds:

* - single bond

+ - double bond

- triple bond

. - ring alternating bond (e.g., benzene)

% - tautomeric bond (e.g., O%%C%%O in carboxylic acids)

Hydrogen atoms are not explicitly included in the diagrams but are understood to occupy any otherwise available bonds.

Tautomeric structures are recognized as equivalent and the percent sign used in the structural diagrams under the following conditions.

M=Q-ZH = HM-Q=Z = H M%%Q%%Z

when:

a). Q = C, N, S, P, Sb, As, Se, Te, Br, Cl, or I with any allowed valence for the individual elements.

b). M and Z = any combination of trivalent N and/or bivalent O, S, Se or Te atoms.

c). The bonds which are involved in the tautomerization may be in an acyclic chain, a ring system, or partly in each.

d). The end points, M and Z, may be in adjacent rings of a fused ring system. However, a nitrogen atom at a fusion point in a fused ring system can not be involved in tautomerization.

e). A deuterium or tritium may replace the migrating hydrogen atom.

f). If more than one of the systems described above are linked through a common atom, the hydrogen may be free to migrate along the chain defining a larger tautomeric system.

The experimental methods were discussed in the preceding section. They are abbreviated as follows:

CLE - Crystal lattice energy
EI - Threshold measurement by non-monoenergetic electron impact
EM - Threshold measurement by monoenergetic electron impact
FAG - Flowing afterglow
FI - Field ionization threshold
ICR - Ion cyclotron resonance
MS - High pressure mass spectrometry
PI - Threshold measurement by photoionization
TC - Theoretical calculation

Following the table of measurements in molecular formula order, Section 4, there are a number of indexes:

a). The gas phase basicity index in which the file is ordered in increasing order of gas phase basicity, with numerical values arbitrarily given to four significiant figures for purposes of ordering. The page number refers to the main body of information, Section 4.

b). The proton affinity index, structured in the same fashion.

c,d,e). Additional indices are provided for molecular formula, CAS Registry Number and compound name. The compound name index includes a number of synonyms in addition to the names adopted in the 8th and 9th collective indices.

Ar	CAS REGN : 7440-37-1
AR	
Argon (8CI9CI)	
PA (exp) : <100.+/-.5 kcal/mol	Temperature :
Roche, A. E., Sutton, M. M., Bohme, D. K., and Schiff, H. I., Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. I. Relative Proton Affinities, J. Chem. Phys. 55, 5480 (1971).	
Method used : FAG Bracketing relative to O2.	

AsH3	CAS REGN : 7784-42-1
AS	
Arsine (8CI9CI)	
GB (exp) : 172.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

BF2H	CAS REGN : 13709-83-6
F**B**F	
Borane, difluoro- (8CI9CI)	
PA (exp) : 115+/-14 kcal/mol	Temperature : 85 K
Pierce, R. C., and Porter, R. F., Ion-Molecule Chemistry of BF3 and HBF2 in Hydrogen, Inorg. Chem. 14, 1087 (1975).	
Method used : MS Bracketing relative to CH4 and H2.	

BF3	CAS REGN : 7637-07-2
F**B**F * * F	
Borane, trifluoro- (9CI) Boron fluoride (BF3) (8CI)	
PA (exp) : 115+/-14 kcal/mol	Temperature : 85 K
Pierce, R. C., and Porter, R. F., Ion-Molecule Chemistry of BF3 and HBF2 in Hydrogen, Inorg. Chem. 14, 1087 (1975).	
Method used : MS Bracketing relative to CH4 and H2.	

B2H6	CAS REGN : 19287-45-7

```
H**B
*  *
*  *
B**H
```

Diborane(6) (8CI9CI)

PA (exp) : 147+/-4 kcal/mol	Temperature : 79-86 K

Pierce, R. C., and Porter, R. F.,
Low-Temperature Chemical Ionization Mass Spectrometry
of Boron Hydrides. The Proton Affinities of Diborane
and Tetraborane(10),
J. Am. Chem. Soc. 95, 3849 (1973).

Method used : MS
Observed reaction C2H9+ + B2H6->2CH4 + B2H7+.
Reaction B2H7+ ->B2H5+ + H2 has delta
H formation = 3.0+/-.3.
Based on delta H formation(B2H5+) = 232.

B3H5N3	CAS REGN : Not available

```
   B**N
  *    *
 *      *
N        B
 *      *
  *    *
   B**N
```

.beta.-Borazinyl radical

PA (exp) : 193+/-2 kcal/mol	Temperature :

DeStefano, A. J., and Porter, R. F.
Ion-Molecule Reactions of Cyclic Borazine Cations.
Thermodynamic and Kinetic Considerations,
J. Phys. Chem. 80, 2818 (1976).

Method used : MS
Bracketing relative to HCO2C2H5 and (CH3)2CO. The reactant ions are generated by photon impact

B3H6N3	CAS REGN : 6569-51-3

```
   B**N
  *    *
 *      *
N        B
 *      *
  *    *
   B**N
```

Borazine (8CI9CI)

PA (exp) : 199+/-4 kcal/mol	Temperature :

Betowski, L. D., Solmon, J. J., and Porter, R. F.,
The Proton Affinity of Borazine,
Inorg. Chem. 11, 424 (1972).

Method used : MS
Bracketing relative to C4H6(2-Butyne) and NH3

B4H8	CAS REGN : 12007-71-5

```
B***B
*   *
*   *
B***B
```

Tetraborane(8)

PA (exp) : 187+/-7 kcal/mol	Temperature : 375 K

Solmon, J. J., and Porter, R. F.,
Chemical Ionization Mass Spectrometry of Selected
Boron Hydrides,
J. Am. Chem. Soc. 94, 1443 (1972).

Method used : MS
Bracketing relative to C3D6 and (CH3)2CO.

B4H10	CAS REGN : 18283-93-7

```
H*****B*****H
 *   * *   *
  * *   * *
   B*****B
  * *   * *
 *   * *   *
H*****B*****H
```

Tetraborane(10) (8CI9CI)

PA (exp) : 144+/-5 kcal/mol	Temperature : 140-300 K

Pierce, R. C., and Porter, R. F.,
Low-Temperature Chemical Ionization Mass Spectrometry
of Boron Hydrides. The Proton Affinities of Diborane
and Tetraborane(10),
J. Am. Chem. Soc. 95, 3849 (1973).

Method used : MS
Based on delta H formation(B2H5+) and estimating delta S.
Equilibrium of B2H5+ + B2H6 -> B4H11+.

B5H9	CAS REGN : 19624-22-7

```
H*****B*****H
 *   ***   *
  * * * * *
   B**B**B
  * * * * *
 *   ***   *
H*****B*****H
```

Pentaborane(9) (8CI9CI)

PA (exp) : 172+/-2 kcal/mol	Temperature : 373~3 K

Solmon, J. J., and Porter, R. F.,
Chemical Ionization Mass Spectrometry of Selected
Boron Hydrides,
J. Am. Chem. Soc. 94, 1443 (1972).

Method used : MS
Based PA (H2O) = 170.3.
Bracketing relative to H2O and H2S.

BrH	CAS REGN : 10035-10-6
BR	
Hydrobromic acid (8CI9CI)	
PA (exp) : 141+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Absolute PA value estimated by assuming that for reaction RH+ + RH -> RH2+ + R; the delta H ~5X TC. TC = measured translational energy of the products.	

CBrN	CAS REGN : 506-68-3
N##C**BR	
Cyanogen bromide (8CI9CI)	
PA (exp) : 179+/-3 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to AsH3, HCO2H and F2CHCH2OH	

CCIN	CAS REGN : 506-77-4
N##C**CL	
Cyanogen chloride (8CI9CI)	
PA (exp) : 177+/-3 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Equilibrium relative to F2CH2CH, OH and HCHO	
GB (exp) : 169.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.4+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

CCl2	CAS REGN : 1605-72-7
CL*C**CL	
Methylene, dichloro- (8CI9CI)	
PA (exp) : 194.7+/-4 kcal/mol	Temperature : 325 K
Ausloos, P., and Lias, S. G. The Proton Affinity of Dichlorocarbene, To be published in J. Am. Chem. Soc.	
Method used : ICR Bracketing relative to Me2O and Et2O; scale based on PA (NH3) = 202.8	
PA (exp) : 200.4+/-1.5 kcal/mol	Temperature : 300 K
Lias, S. G., and Ausloos, P. Reactions of CCl2H+ and CF2H+ with Organic and Inorganic Compounds: Proton Affinities and Heats of Formation of CCl2 and CF2, Intern. J. Mass Spectrom. Ion Phys. 22, 135 (1976).	
Method used : ICR Bracketing relative to NH3 and (CH3)2S	

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GB not calculated for this reference	
PA (exp) : 208.3+/-2 kcal/mol	Temperature : 300 K
Levi, B. A., Taft, R. W., and Hehre, W. J. Dichlorcarbene, J. Am. Chem. Soc. 99, 8454 (1977).	
Method used : ICR Calculated entropy Bracketing relative to CF3CH2CH2NH2 and C6H5NH2; scale based on NH3	
PA (exp) : 209+/-2 kcal/mol	Temperature : 300 K
Levi, B. A., Taft, R. W., and Hehre, W. J. Dichlorocarbene, J. Am. Chem. Soc. 99, 8454 (1977).	
Method used : ICR Calculated entropy The deuterium affinity determined by bracketing techniques relative to 2-CF3 Pyridine and CF3(CH2)2NH2; scale based on NH3	

CF2	CAS REGN : 2154-59-8
F**C**F	
Methylene, difluoro- (8CI9CI)	
PA (exp) : 178.5+/-1 kcal/mol	Temperature : 300 K
Lias, S. G., and Ausloos, P. Reactions of CCl2H+ and CF2H+ with Organic and Inorganic Compounds: Proton Affinities and Heats of Formation of CCl2 and CF2, Intern. J. Mass Spectrom. Ion Phys. 22, 135 (1976).	
Method used : ICR Bracketing relative to H2S and HCOOH and also observing the following: CD5+ + CF2HCL -> CD4 + DCl + CF2H+ and CD5+ + CF3H -> CD4 + DF + CF2H+. Scale based on PA (H2O) = 170.1 kcal/mol	

CF4	CAS REGN : 75-73-0

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   F
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F**C**F
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   F
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Methane, tetrafluoro- (9CI)
Carbon tetrafluoride (8CI)

PA (exp) : 121+/-4 kcal/mol	Temperature : 300 K

Roche, A. E., Sutton, M. M., Bohme, D. K., and Schiff, H. I., Determination of Proton Affinity from the Kinetics of Proton Transfer Reactions. I. Relative Proton Affinities, J. Chem. Phys. 55, 5480 (1971).

Method used : FAG
Bracketing relative to CH4 and N2.

PA (exp) : 121+/-5 kcal/mol	Temperature : 298 K

Blint, R. J., McMahon, T. B., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities, J. Am. Chem. Soc. 96, 1269 (1974).

Method used : ICR
Bracketing relative to CH4. Using IP of H and CF4 and also HA of CF4+.

CHF3	CAS REGN : 75-46-7
F**C**F * * F	
Methane, trifluoro- (8CI9CI)	
PA (exp) : 147+/-5 kcal/mol	Temperature : 298 K
Blint, R. J., McMahon, T. B., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities, J. Am. Chem. Soc. 96, 1269 (1974).	
Method used : ICR Bracketing relative to CH3F. Using IP of H and CH3F, also HA (CH3F+).	

CHN	CAS REGN : 74-90-8
C##N	
Hydrocyanic acid (8CI9CI)	
GB (exp) : 166.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.5+/-2 kcal/mol	Temperature : 300 K
Freeman, C. G., Harland, P. W., and McEwan, M. J. The Equilibrium H3S+ + HCN = H2CN+ + H2S and the Relative Proton Affinities of HCN and H2S, Intern. J. Mass Spectrom. Ion Phys. 27, 77 (1978).	
Method used : FAG Equilibrium relative to H2S; scale based on NH3	
PA (exp) : 139 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Estimated delta H = 5X translational energy of the product of reaction RH+ + RH -> RH2+ + R	

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GB (exp) : 166.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.5+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

CH2F2	CAS REGN : 75-10-5

F**C**F

Methane, difluoro- (8CI9CI)

PA (exp) : 147+/-5 kcal/mol	Temperature : 298 K

Blint, R. J., McMahon, T. B., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Fluoromethanes by Ion Cyclotron Resonance Spectroscopy. New Techniques for the Determination of Carbonium Ion Stabilities, J. Am. Chem. Soc. 96, 1269 (1974).

Method used : ICR
Bracketing relative to CH3F and CO. Using IP of H and CH2F2, also HA (CH2F2+).

CH2N2	CAS REGN : 334-88-3
N++N++C	
Methane, diazo- (8CI9CI)	
PA (exp) : 207+/-5 kcal/mol	Temperature : 300 K
Foster, M. S., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance, J. Am. Chem. Soc. 94, 2425 (1972).	
Method used : ICR Bracketing relative to NH3 and CH3NH2	

CH2O	CAS REGN : 50-00-0
C++O	
Formaldehyde (8CI9CI)	
PA (exp) : 162+/-3 kcal/mol	Temperature :
Harrison, A. G., Ivko, A., and Van Raalte, D., Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds, Can. J. Chem. 44, 1625 (1966).	
Method used : EI Electron impact fragmentation (various molecules).	

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PA (exp) : 169+/-1 kcal/mol	Temperature : 298 K

Refaey, K. M. A., and Chupka, W. A.,
Photoionization of the Lower Aliphatic Alcohols
with Mass Analysis,
J. Chem. Phys. 48, 5205 (1968).

Method used : PI
Appearance potential by IP fragmentation of CH3OH

PA (exp) : 170 kcal/mol	Temperature :

Lossing, F. P.
Heats of Formation of Some Isomeric [CnH2n + 1O]+
Ions. Substitutional Effects on Ion Stability,
J. Am. Chem. Soc. 99, 7526 (1977).

Method used : EM
Electron impact fragmentation (various molecules)
using EM. delta Hf(H+) = 365.7

GB (exp) : 167.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.6+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,
McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of
Compounds between Water and Ammonia from Pulsed Ion
Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

CH2O2	CAS REGN : 64-18-6
O%%C%%O	
Formic acid (8CI9CI)	
PA (exp) : 178+/-4 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH3OH and H2S.	
PA (exp) : 186.8 kcal/mol	Temperature :
Goldenfeld, I. V., Korostyshevsky, I. Z., and Mischanchuk, B. G., Analysis of Field Ion Energies in a Mass Spectrometer, Int. J. Mass Spectrom. Ion Phys. 13, 297 (1974).	
Method used : FI PA derived from field appearance potential. Correction for neutral particles potential energy	

Continued on next page

PA (exp) : 179+/-3 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Heats of Formation of Protonated Cyclopropane,
Methylcyclopropane, and Ethane,
J. Am. Chem. Soc. 94, 5347 (1972).

Method used : MS
Correction for path degeneracy.
Equilibrium; scale based on CH3CH=CH2.

GB (exp) : 162.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 178.9+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds
between Water and Ammonia and Substituted Benzenes from
a Continuous Ladder of Proton Transfer Equilibria
Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 171.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

CH3Br	CAS REGN : 74-83-9
BR*C	
Methane, bromo- (8CI9CI)	
PA (exp) : 163 kcal/mol	Temperature : 300 K

Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).

Method used : ICR
Bracketing and using also IP's of H and CH3Br and HA(CH3BR+).

CH3Cl	CAS REGN : 74-87-3
C**CL	
Methane, chloro- (8CI9CI)	
PA (exp) : <170.3 kcal/mol	Temperature :
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds,. J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to H2O.	
PA (exp) : 164+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Absolute PA value estimated by assuming that for reaction RH+ + RH ->R + RH2+ the delta H ~5X TC. TC = measured translational energy of the products	

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PA (exp) : ~160 kcal/mol	Temperature : 300 K

Beauchamp, J. L., Holtz, D., Woodgate, S. D.,
and Patt, S. L.,
Thermochemical Properties and Ion-Molecule Reactions
of the Alkyl Halides in the Gas Phase by Ion Cyclotron
Resonance Spectroscopy,
J. Am. Chem. Soc. 94, 2798 (1972).

Method used : ICR
Bracketing and using also IP's of H and CH3CL
and HA(CH3CL+).

CH3F	CAS REGN : 593-53-3

C**F

Methane, fluoro- (8CI9CI)

PA (exp) : 151+/-5 kcal/mol	Temperature : 298 K

Beauchamp, J. L., Holtz, D., Woodgate, S. D.,
and Patt, S. L.,
Thermochemical Properties and Ion-Molecule Reactions
of the Alkyl Halides in the Gas Phase by Ion Cyclotron
Resonance Spectroscopy,
J. Am. Chem. Soc. 94, 2798 (1972).

Method used : ICR
Using also the IP's of H
and CH3F and HA of CH3F+.

CH3I	CAS REGN : 74-88-4
C**I	
Methane, iodo- (8CI9CI)	
PA (exp) : 174+/-3 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and CH3I and HA(CH3I+).	

CH3NO2	CAS REGN : 75-52-5

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O++N**C
   +
   +
   O
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Methane, nitro- (8CI9CI)

PA (exp) : ~182 kcal/mol	Temperature : 300 K

McAllister, T., and Pitman, P.
Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane,
Intern. J. Mass Spectrom. Ion Phys. 19, 241 (1976).

Method used : ICR
Bracketing relative to CH3OH and (CH3)2CO

PA (exp) : 182+/-2 kcal/mol	Temperature : 300 K

Kriemler, P., and Buttrill, S. E., Jr.,
Ion-Molecule Reactions and the Proton Affinities of the Nitroalkanes. I. Nitro methane and nitroethane,
J. Am. Chem. Soc. 95, 1365 (1973).

Method used : ICR
Bracketing relative to CH3OH.

CH3NO2	CAS REGN : 624-91-9
O++N**O**C	
Nitrous acid, methyl ester (8CI9CI)	
PA (exp) : 190.3+/-3 kcal/mol	Temperature : 300 K
McAllister, T., and Pitman, P. Ion-Molecule Reactions and Proton Affinities of Methyl Nitrite and Nitromethane, Intern. J. Mass Spectrom. Ion Phys. 19, 241 (1976).	
Method used : ICR Bracketing relative to C2H5OH and (CH3)2CO	

CH4	CAS REGN : 74-82-8
C	
Methane (8CI9CI)	
PA (exp) : 127+/-2 kcal/mol	Temperature : 78,300 K
Chupka, W. A., and Berkowitz, J., Photoionization of Methane: Ionization Potential and Proton Affinity of CH4, J. Chem. Phys. 54, 4256 (1971).	
Method used : PI From PI-efficiency curve of CH5+ in CH4.	

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PA (exp) : 126+/-1 kcal/mol	Temperature : 483+/-10 K

Munson, M. S. B., and Field, F. H.,
Reactions of Gaseous Ions. XV. Methane + 1% Ethane
and Methane + 1% Propane,
J. Am. Chem. Soc. 87, 3294 (1965).

Method used : MS
Observed reactions: $CH_4^+ + CH_4 \rightarrow CH_5^+ + CH_3$,
$CH_5^+ + C_2H_6 \rightarrow C_2H_5^+ + H_2 + CH_4$.

PA (exp) : 131.4 kcal/mol	Temperature : 298 K

Schiff, H. I., and Bohme, D. K.,
Flowing Afterglow Studies at York University,
Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).

Method used : FAG
Equilibrium relative to N_2O, delta S
estimated. Based on PA (N_2O) which is derived
from calculated PA (CO).

PA (exp) : 130.5 kcal/mol	Temperature : 340 K

Kasper, S. F., and Franklin, J. L.,
Ion-Molecule Reactions in the System CO_2-CH_4,
J. Chem. Phys. 56, 1156 (1972).

Method used : MS
Entropy change assumed zero
Equilibrium relative to CO_2; found delta
G = -1.35 Kcal/mol. Based on CO_2 with PA = 129.1.
(Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975)).

CH4O	CAS REGN : 67-56-1
C**O	
Methanol (8CI9CI)	
PA (exp) : 182+/-3 kcal/mol	Temperature :
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH3CHO and HCOOH.	
PA (exp) : 179.0+/-2 kcal/mol	Temperature : 299-329 K
Wei, L. Y., and Bone, L. I., Ion-Molecule Reactions in Methanol and Hydrogen Sulfide, J. Phys. Chem. 78, 2527 (1974).	
Method used : MS Equilibrium relative to H2S Van't Hoff plot	

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PA (exp) : 182 kcal/mol	Temperature :

Haney, M. A., and Franklin, J. L.,
Mass Spectrometric Determination of the Proton Affinities of Various Molecules,
J. Phys. Chem. 73, 4328 (1969).

Method used : MS
Delta H estimated = 5X total translational energy of the products of RH+ + RH -> RH2+ + R

GB (exp) : 166.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.1+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

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GB (exp) : 174.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 182.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

CH4S	CAS REGN : 74-93-1
C**S	
Methanethiol (8CI9CI)	
GB (exp) : 177.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 185.3+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on CH3CHO Entropy change assumed zero	

Continued on next page

PA (exp) : 199+/-10 kcal/mol	Temperature :

Hobrock, B. G. and Kiser, R. W.,
Electron Impact Investigations of Sulfur Compounds.
II. 3-Methyl-2-Thiabutane, 4-Thia-1-Pentene, and
3,4-Dithiahexane,
J. Phys. Chem. 67, 648 (1963).

Method used : EI
Appearance potential by electron impact of sulfur
compounds.

GB (exp) : 178.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 185.9+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,
McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of
Compounds between Water and Ammonia from Pulsed Ion
Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

CH5N	CAS REGN : 74-89-5
C**N	
Methanamine (9CI) Methylamine (8CI)	
GB (exp) : 202.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 211 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Estimated delta H = 5X translational energy of the product of reaction RH+ + RH -> RH2+ + R	

Continued on next page

GB (exp) : 205.7+/-3 kcal/mol	Temperature : 298 K
PA (exp) : 213.7+/-3 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T. Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 195.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 213.1+/-2 kcal/mol	Temperature : 600 K
Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton- Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	

CH5P	CAS REGN : 593-54-4
C**P	
Phosphine, methyl- (8CI9CI)	
GB (exp) : 193.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 201.8+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

CO	CAS REGN : 630-08-0
C##O	
Carbon monoxide (8CI9CI)	
PA (exp) : 143+/-2 kcal/mol	Temperature :
Matthews, C. S., and Warneck, P., Heats of Formation of CHO+ and C3H3+ by Photoionization, J. Chem. Phys. 51, 854 (1969).	
Method used : PI Appearance potential by photoionization. PA value derived from delta H formation(HCO+).	
PA (exp) : 142.7+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Excess Energies in Mass Spectra of some Oxygen-Containing Organic Compounds, Trans. Faraday Soc. 65, 1794 (1969).	
Method used : MS Appearance potential by electron impact from HCOOH, CH3CHO and C2H3CHO. Correction for excess energy.	

CO2	CAS REGN : 124-38-9
O++C++O	
Carbon dioxide (8CI9CI)	
PA (exp) : 130.7+/-1 kcal/mol	Temperature :
Warneck, P. Heat of Formation of the HCO Radical, Z. Naturforsch. 29, 350 (1974).	
Method used : PI Appearance potential by photoionization. delta Hf(H+) = 365.7	
PA (exp) : 129.1 kcal/mol	Temperature : 298 K
Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).	
Method used : FAG Calculated entropy. Equilibrium; scale based on CO VALUE	

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PA (exp) : 124+/-2 kcal/mol	Temperature : 300 K

Meot-Ner (Mautner), M., and Field, F.
Proton Affinities and Cluster Ion Stabilities in
CO2 and CS2. Applications in Martian Ionspheric
Chemistry,
J. Chem. Phys. 66, 4527 (1977).

Method used : MS
Van't Hoff plot
Equilibrium; scale based on PA (CH4) = 126.8

GB (exp) : 123+/-3 kcal/mol	Temperature : 300 K
PA (exp) : 124+/-3 kcal/mol	Temperature : 300 K

Meot-Ner (Mautner), M., and Field, F. H.
Proton Affinities and Cluster Ion Stabilities in
CO2 and CS2. Application in Martian Ionspheric
Chemistry,
J. Chem. Phys. 66, 4527 (1977).

Method used : MS
Calculated entropy
The measurements done in the temperature range of
400-650K. Using the Hoff plot the delta H and delta S at
300K were derived. Using PA (CH4)-126.8

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PA (exp) : 123+/-3 kcal/mol	Temperature : 800 K

Fehsenfeld, F. C., Lindinger, W., Schiff, H. I., Hemsworth, R. S., and Bohne, D. K. Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. VI. The Relative Proton Affinities of N2, Xe, and CO2, J. Chem. Phys. 64, 4887 (1976).

Method used : FAG
Van't Hoff plot
Equilibrium relative to N2 and Xe; scale based on PA (N2) = 112.6
Van't Hoff plot

CS2	CAS REGN : 75-15-0
S++C++S	
Carbon disulfide (8CI9CI)	
GB (exp) : 165.7+/-2.5 kcal/mol	Temperature : 300 K
PA (exp) : 168+/-2.5 kcal/mol	Temperature : 300 K

Meot-Ner (Mautner), M., and Field, F. H. Proton Affinities and Cluster Ion Stabilities in CO2 and CS2. Applications in Martian Ionspheric Chemistry, J. Chem. Phys. 66, 4527 (1977).

Method used : MS
Calculated entropy
The measurements done in the temperature range of 400-650K. Using the Hoff plot the delta H and delta S at 300K were derived. Equilibrium, scale based on NH3

C2Cl3N	CAS REGN : 545-06-2

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   CL
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CL*C**C##N
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   *
   CL
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Acetonitrile, trichloro- (8CI9CI)

GB (exp) : 169.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.5+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2D6O	CAS REGN : 17222-37-6
C**O**C	
Methane-d3, oxybis- (9CI) (Methyl ether)-d6 (8CI)	
GB (exp) : ~186 kcal/mol	Temperature : 374 K
Blair, A. S., and Harrison, A. G., Bimolecular Reactions of Trapped Ions. V. Ionic Chemistry of Simple Oxygen-containing Molecules, Can. J. Chem. 51, 703 (1972).	
Method used : MS Equilibrium relative to CH3CHO. Found delta G ~3.	

C2HF3	CAS REGN : 359-11-5

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F**C++C**F
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   *
   F
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Ethene, trifluoro- (9CI)
Ethylene, trifluoro- (8CI)

PA (exp) : 172+/-2 kcal/mol	Temperature : 300 K

Ridge, D. P.,
Gas Phase Proton Affinities of Several Fluoroethylenes,
J. Am. Chem. Soc. 97, 5670 (1975).

Method used : ICR
Bracketing relative to H2O and H2S.

C2HF3O2	CAS REGN : 76-05-1

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   F
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F**C**C%%O
   *  %
   *  %
   F  O
```

Acetic acid, trifluoro- (8CI9CI)

PA (exp) : 172+/-2 kcal/mol	Temperature : 323-373 K

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to H2S and H2O

GB (exp) : 154.7+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 171.9+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

Continued on next page

GB (exp) : 165.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 173.3+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2H2ClN	CAS REGN : 107-14-2

CL*C**C##N

Acetonitrile, chloro- (8CI9CI)

GB (exp) : 173.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2H2F2	CAS REGN : 75-38-7

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F**C++C
   *
   *
   F
```

Ethene, 1,1-difluoro- (9CI)
Ethylene, 1,1-difluoro- (8CI)

PA (exp) : 178+/-4 kcal/mol	Temperature : 300 K

Ridge, D. P.,
Gas Phase Proton Affinities of several Fluoroethylenes,
J. Am. Chem. Soc. 97, 5670 (1975).

Method used : ICR
Bracketing relative to C2H5I and CH3OH

PA (exp) : 174.8 kcal/mol	Temperature : 298 K

Williamson, A. D., LeBrenton, P. R., and
Beauchamp, J. L.,
Photoionization Mass Spectrometry of 2-Fluoropropane
and 2,2-Difluoropropane. A Novel Determination of the
Proton Affinity of Vinyl Fluoride and 1,1-Difluoro-
ethylene,
J. Am. Chem. Soc. 98, 2705 (1976).

Method used : PI
Appearance potential by phtotionization of (CH3)2CF2.

C2H2F2	CAS REGN : 1630-77-9
F**C++C**F	
Ethene, 1,2-difluoro-, (Z)- (9CI) Ethylene, 1,2-difluoro-, (Z)- (8CI)	
PA (exp) : 166+/-4 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to C2H5F and H2O.	

C2H2F2	CAS REGN : 1630-78-0
F**C++C**F	
Ethene, 1,2-difluoro-, (E)- (9CI) Ethylene, 1,2-difluoro-, (E)- (8CI)	
PA (exp) : 167+/-4 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to C2H5F and H2O.	

C2H2O	CAS REGN : 463-51-4
O++C++C	
Ethenone (9CI) Ketene (8CI)	
PA (exp) : 194.1+/-1 kcal/mol	Temperature : 350 K
Ausloos, P., and Lias, S. G. The Proton Affinity of Ketene and the Heat of Formation of CH3CO+, Chem. Phys. Letters 51, 53 (1977).	
Method used : ICR Equilibrium; scale based on PA (iso-C4H8) = 193.5+/-1	
PA (exp) : 195.9+/-2 kcal/mol	Temperature : 300 K
Vogt, J., Williamson, A. D., and Beauchamp, J. L. Properties and Reactions of Ketene in the Gas Phase by Ion Cyclotron Resonance Spectroscopy and Photoionization Mass Spectrometry. Proton Affinity, Site Specificity of Protonation, and Heat of Formation of Ketene, J. Am. Chem. Soc. 100, 3478 (1978).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H3ClO2	CAS REGN : 79-11-8

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O%%C**C**CL
   %
   %
   O
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Acetic acid, chloro- (8CI9CI)

GB (exp) : 166.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 184+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C2H3Cl3O	CAS REGN : 115-20-8

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   CL
   *
   *
CL*C**C**O
   *
   *
   CL
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Ethanol, 2,2,2-trichloro- (8CI9CI)

GB (exp) : 171.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 179+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2H3F	CAS REGN : 75-02-5
F**C++C	
Ethene, fluoro- (9CI) Ethylene, fluoro- (8CI)	
PA (exp) : 174+/-1 kcal/mol	Temperature : 300 K
Ridge, D. P., Gas Phase Proton Affinities of several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).	
Method used : ICR Bracketing relative to H2S and CH2O.	
PA (exp) : 173.6 kcal/mol	Temperature : 298 K
Williamson, A. D., LeBreton, P. R., and Beauchamp, J. L., Photoionization Mass Spectrometry of 2-Fluoro- propane and 2,2-Difluoropropane. A Novel Determination of Vinyl Fluoride and 1,1-Diflouro- ethylene, J. Am. Chem. Soc. 98, 2705 (1976).	
Method used : PI Appearance potential by photoionization of (CH3)2CHF.	

C2H3FO2	CAS REGN : 144-49-0

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O%%C**C**F
   %
   %
   O
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Acetic acid, fluoro- (8CI9CI)

GB (exp) : 167.3+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 184.5+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C2H3F3O	CAS REGN : 75-89-8

```
   F
   *
   *
F**C**C**O
   *
   *
   F
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Ethanol, 2,2,2-trifluoro- (8CI9CI)

GB (exp) : 164.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 172.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2H3N	CAS REGN : 75-05-8
N##C**C	
Acetonitrile (&CI9CI)	
PA (exp) : 189.5+/-4.5 kcal/mol	Temperature : 298 K
Gray, G. A., Study of Ion-Molecule Reactions and Reaction Mechanisms in Acetonitrile by Ion Cyclotron Resonance, J. Am. Chem. Soc. 90, 6002 (1968).	
Method used : ICR Bracketing relative to CH3CHO and (CH3)2CO	
PA (exp) : 186+/-1 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Translational energy of RH2+ has been measured assuming delta H = 5X translational energy for reaction RH+ + RH -> RH2+ + R	

Continued on next page

GB (exp) : 179.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 171.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 187.4+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C2H3NS	CAS REGN : 556-61-6
S++C++N**C	
Methane, isothiocyanato- (9CI) Isothiocyanic acid, methyl ester (8CI)	
PA (exp) : 189+/-6 kcal/mol	Temperature : 300 K
McAllister, T., Ion-Molecule Reactions and Proton Affinities of Methyl Thio- and Isothiocyanate, Int. J. Mass Spectrom. Ion Phys. 15, 303 (1974).	
Method used : ICR Bracketing relative to (CH3)2CO and 1-C4H8.	

C2H3NS	CAS REGN : 556-64-9
N##C**S**C	
Thiocyanic acid, methyl ester (8CI9CI)	
PA (exp) : 189+/-6 kcal/mol	Temperature : 300 K
McAllister, T., Ion-Molecule Reactions and Proton Affinities of Methyl Thio- and Isothiocyanate, Int. J. Mass Spectrom. Ion Phys. 15, 303 (1974).	
Method used : ICR Bracketing relative to (CH3)2CO and 1-C4H8.	

C2H4	CAS REGN : 74-85-1
C++C	
Ethene (9CI) Ethylene (8CI)	
PA (exp) : 160.6 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P., Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C2H5+ using EM.	

C2H4F2O	CAS REGN : 359-13-7

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F**C**C**O
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   F
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Ethanol, 2,2-difluoro- (8CI9CI)

GB (exp) : 170.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.9+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2H4F3N	CAS REGN : 753-90-2

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F**C**C**N
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   F
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Ethanamine, 2,2,2-trifluoro- (9CI)
Ethylamine, 2,2,2-trifluoro- (8CI)

GB (exp) : 188.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 197.9+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.3+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C2H4N2	CAS REGN : 540-61-4
N**C**C##N	
Acetonitrile, amino- (8CI9CI)	
PA (exp) : ~197 kcal/mol	Temperature : 300 K
Taagepera, M., Hehre, W. J., Topsom, R. D., and Taft, R. W. Calculation of Polar Substituent Parameters by ab initio Molecular Orbital Methods. Proton Affinities of Substituted Primary Amines, J. Am. Chem. Soc. 98, 7438 (1976).	
Method used : ICR Equilibrium; scale based on NH3	

C2H4O	CAS REGN : 75-07-0
O++C**C	
Acetaldehyde (8CI9CI)	
PA (exp) : 184+/-3 kcal/mol	Temperature :
Harrison, A. G., Ivko, A., and Van Raalte, D., Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds, Can. J. Chem. 44, 1625 (1966).	
Method used : EI Electron impact fragmentation	
PA (exp) : 186+/-1 kcal/mol	Temperature : 298 K
Refaey, K. M. A., and Chupka, W. A., Photoionization of the Lower Aliphatic Alcohols with Mass Analysis, J. Chem. Phys. 48, 5205 (1968).	
Method used : PI Appearance potential by IP fragmentation of C2H5OH.	

Continued on next page

PA (exp) : 189.4 kcal/mol	Temperature : 298 K
Lossing, F. P. Heats of Formation of Some Isomeric [CnH2n + 1O]+ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).	
Method used : EM Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7	
GB (exp) : 177.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 185+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

Continued on next page

GB (exp) : 169.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 185.4+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C2H4O	CAS REGN : 75-21-8

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   O
  * *
 *   *
C*****C
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Oxirane (9CI)
Ethylene oxide (8CI)

PA (exp) : 185+/-4 kcal/mol	Temperature :

Beauchamp, J. L., and Dunbar, R. C.,
Identification of C2H5O+ Structural Isomers by Ion Cyclotron Resonance Spectroscopy,
J. Am. Chem. Soc. 92, 1477 (1970).

Method used : ICR
Bracketing relative to CH3OH and (CH3)2O

C2H4O2	CAS REGN : 64-19-7
O%%C**C % % O	
Acetic acid (8CI9CI)	
PA (exp) : 188+/-3 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Equilibrium; scale based on NH3	
GB (exp) : 171.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 188.2+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

Continued on next page

GB (exp) : 179.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H4O2	CAS REGN : 107-31-3
O++C**O**C	
Formic acid, methyl ester (8CI9CI)	
PA (exp) : 188+/-3 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (CH3)2O and CH3CHO	

Continued on next page

GB (exp) : 179.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on CH3CHO Entropy change assumed zero	
GB (exp) : 179.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

Continued on next page

GB (exp) : 172.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 187.8+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C2H5Br	CAS REGN : 74-96-4
C**C**BR	
Ethane, bromo- (8CI9CI)	
PA (exp) : 171+/-2 kcal/mol	Temperature : 300 K

Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L.,
Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy,
J. Am. Chem. Soc. 94, 2798 (1972).

Method used : ICR
Bracketing and using also IP's of H and C2H5BR and assuming HA(CH3BR+)=HA(C2H5BR+).

C2H5Cl	CAS REGN : 75-00-3
CL*C**C	
Ethane, chloro- (8CI9CI)	
PA (exp) : 170+/-2 kcal/mol	Temperature :
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and C2H5CL and HA(CH3CL+)=HA(C2H5CL+).	

C2H5F	CAS REGN : 353-36-6
F**C**C	
Ethane, fluoro- (8CI9CI)	
PA (exp) : 165+/-5 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also the IP's of H and C2H5F and assuming HA(CH3F+) = HA(C2H5F+).	

C2H5F2N	CAS REGN : 430-67-1
F**C**C**N * * F	
Ethanamine, 2,2-difluoro- (9CI) Ethylamine, 2,2-difluoro- (8CI)	
GB (exp) : 197.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H5I	CAS REGN : 75-03-6
I**C**C	
Ethane, iodo- (8CI9CI)	
PA (exp) : 175 kcal/mol	Temperature : 300 K
Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2798 (1972).	
Method used : ICR Bracketing and using also IP's of H and assuming HA(CH3I+)=HA(C2H5I+).	

C2H5N	CAS REGN : 151-56-4
N * * * * C*****C	
Aziridine (9CI) Ethylenimine (8CI)	
GB (exp) : 204.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 204.9+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

Continued on next page

PA (exp) : 213+/-2 kcal/mol	Temperature : 300 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Proton Affinities, Ionization Potentials, and
Hydrogen Affinities of Nitrogen and Oxygen Bases.
Hybridization Effects,
J. Am. Chem. Soc. 97, 4137 (1975).

Method used : ICR
Equilibrium; scale based on CH3NH2
Van't Hoff plot

C2H5NO	CAS REGN : 60-35-5

N%%C**C
%
%
O

Acetamide (8CI9CI)

GB (exp) : 188.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 205.7+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding
in Proton-Bound Amine Dimers and Proton-Induced
Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Equilibrium; scale based on CH3NH2
Entropy change assumed zero

C2H5NO	CAS REGN : 123-39-7
O%%C%%N**C	
Formamide, N-methyl- (8CI9CI)	
GB (exp) : 195+/-4 kcal/mol	Temperature : 300 K
PA (exp) : 202.8+/-4 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H5NO2	CAS REGN : 79-24-3

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O++N**C**C
   +
   +
   O
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Ethane, nitro- (8CI9CI)

PA (exp) : 186+/-2 kcal/mol	Temperature : 300 K

Kriemler, P., and Buttrill, S. E., Jr.,
Ion-Molecule Reactions and the Proton Affinities
of the Nitroalkanes,
J. Am. Chem. Soc. 95, 1365 (1973).

Method used : ICR
Bracketing relative to CH3CN and CH3CHO.

C2H5NO3	CAS REGN : 625-58-1

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C**C**O**N++O
          +
          +
          O
```

Nitric acid, ethyl ester (8CI9CI)

PA (exp) : 181+/-3 kcal/mol	Temperature : 300 K

Kriemler, P., and Buttrill, S. E., Jr.,
Positive and Negative Ion-Molecule Reactions and
the Proton Affinity of Ethyl Nitrate,
J. Am. Chem. Soc. 92, 1123 (1970).

Method used : ICR
Bracketing relative to cyclo-C6H10 and CH3NO2.

C2H6	CAS REGN : 74-84-0
C**C	
Ethane (8CI9CI)	
PA (exp) : 128+/-1 kcal/mol	Temperature :
Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).	
Method used : MS By applying path degeneracy correction found delta H formation (C2H7+) = 218.8 Equilibrium relative to CH4; assume delta S = 0.	
PA (exp) : 139.6 (1) kcal/mol	Temperature : 300 K
Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C2H7+ Ions and Some Higher Analogues: C3H9+ and C4H11+, J. Am. Chem. Soc. 98, 6119 (1976).	
Method used : MS Based on delta H formation(C2H5+) = 219. Equilibrium of reaction: C2H5+ + H2 -> C2H7+(C-C protonation) (1).	

Continued on next page

PA (exp) : 131.8 (2) kcal/mol	Temperature :

Hiraoka, K., and Kebarle, P.,
Stabilities and Energetics of Pentacoordinated
Carbonium Ions. The Isomeric C2H7+ Ions and Some
Higher Analogues: C3H9+ and C4H11+,
J. Am. Chem. Soc. 98, 6119 (1976).

Method used : MS
Based on delta H formation(C2H5+) = 219
Equilibrium of reaction:
C2H5+ + H2 + H2->C2H7+ + H2(CH protonation) (2).

C2H6FN	CAS REGN : 406-34-8

F**C**C**N

Ethanamine, 2-fluoro- (9CI)
Ethylamine, 2-fluoro- (8CI)

GB (exp) : 201.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C2H6N2	CAS REGN : 4143-41-3
C**N++N**C	
Diazene, dimethyl-, (E)- (9CI) Azomethane, (E)- (8CI)	
GB (exp) : 197.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.5+/-2 kcal/mol	Temperature : 300 K
Foster, M. S., Williamson, A. D., and Beauchamp, J. L., Photoionization Mass Spectrometry of trans-Azomethane, Int. J. Mass Spectrom. Ion Phys. 15, 429 (1974).	
Method used : MS Calculated entropy Equilibrium relative to NH3	
PA (exp) : 206.8+/-5 kcal/mol	Temperature : 300 K
Foster, M. S., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance, J. Am. Chem. Soc. 94, 2425 (1972).	
Method used : ICR Bracketing between NH3 and CH3NH2	

C2H6O	CAS REGN : 64-17-5
O**C**C	
Ethanol (9CI) Ethyl alcohol (8CI)	
PA (exp) : 186+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH3COOH and CH3CHO	
GB (exp) : 178.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 186.2+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on CH3CHO Entropy change assumed zero	

Continued on next page

GB (exp) : 171.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 186.8+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 178.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 186.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H6O	CAS REGN : 115-10-6
C**O**C	
Methane, oxybis- (9CI) Methyl ether (8CI)	
PA (exp) : 190+/-4 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to I-C4H8 and CH3CHO; Scale based on NH3	
PA (exp) : 189 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Delta H assume = 5X translational energy of the products of reaction RH + RH+ -> RH2+ + R.	

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GB (exp) : 181.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 189.1+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on MECHO Entropy change assumed zero	
GB (exp) : 174.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 189.3+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

Continued on next page

GB (exp) : 182.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 193.3 kcal/mol	Temperature : 300 K
Hiraoka, K., Grimsrud, E. P., and Kebarle, P., Gas Phase Ion Equilibria Studies of the Hydrogen Ion in Water-Dimethyl Ether and Methanol-Dimethyl, J. Am. Chem. Soc. 96, 3359 (1974).	
Method used : MS Van't Hoff plot Equilibrium relative to H2O. Delta G determined by means of thermodynamic cycles involving mixed clusters.	

C2H6OS	CAS REGN : 67-68-5

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C**S**C
   +
   +
   O
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Methane, sulfinylbis- (9CI)
Methyl sulfoxide (8CI)

GB (exp) : 200.9+/-2.5 kcal/mol	Temperature : 300 K
PA (exp) : 208.3+/-2.5 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 184+/-3 kcal/mol	Temperature : 300 K

McAllister, T.
Ion Cyclotron Resonance Mass Spectroscopy of Dimethyl Sulfoxide,
Intern. J. Mass Spectrom. Ion Phys. 25, 353 (1977).

Method used : ICR
Bracketing relative to CH3OH and EtOH.

C2H6S	CAS REGN : 75-08-1
S**C**C	
Ethanethiol (8CI9CI)	
GB (exp) : 180.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H6S	CAS REGN : 75-18-3
C**S**C	
Methane, thiobis- (9CI) Methyl sulfide (8CI)	
GB (exp) : 190.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H7N	CAS REGN : 75-04-7
N**C**C	
Ethanamine (9CI) Ethylamine (8CI)	
GB (exp) : 205.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.0+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 205.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 214.3+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C2H7N	CAS REGN : 124-40-3
C**N**C	
Methanamine, N-methyl- (9CI) Dimethylamine (8CI)	
GB (exp) : 209.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 209.5+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.7+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

Continued on next page

GB (exp) : 203.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 220.6+/-2 kcal/mol	Temperature : 600 K

Briggs, J. P., Yamdagni, R., and Kebarle, P.,
Intrinsic Basicities of Ammonia, Methylamines,
Anilines, and Pyridine from Gas-Phase Proton-
Exchange Equilibria,
J. Am. Chem. Soc. 94, 5128 (1972).

Method used : MS
Entropy change assumed zero
Equilibrium; scale based on NH3

C2H7P	CAS REGN : 676-59-5
C**P**C	
Phosphine, dimethyl- (8CI9CI)	
GB (exp) : 205.6+/-2 kcal/mol	Temperature : 298 K

Taft, R. W.,
Proton-Transfer Reactions,
Ed. E. F. Caldin and V. Gold,
(John Wiley and Sons, New York, 1975) Ch. 2.

Method used : ICR
Equilibrium; scale based on NH3

C2H8N2	CAS REGN : 57-14-7
C**N**C * * N	
Hydrazine, 1,1-dimethyl- (8CI9CI)	
GB (exp) : 209.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C2H8N2	CAS REGN : 107-15-3
N**C**C**N	
1,2-Ethanediamine (9CI) Ethylenediamine (8CI)	
GB (exp) : 213.60+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.50+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 215.50+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 227.50+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

C3D9N	CAS REGN : 13960-80-0
C**N**C * * C	
Methan-d3-amine, N,N-di(methyl-d3)- (9CI) Trimethylamine-d9 (8CI)	
GB (exp) : 214.00+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

C3H2N2	CAS REGN : 109-77-3
N##C**C**C##N	
Propanedinitrile (9CI) Malononitrile (8CI)	
GB (exp) : 169.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 177.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H3F3O2	CAS REGN : 431-47-0

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          F
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          *
C**O**C**C**F
      +   *
      +   *
      O   F
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Acetic acid, trifluoro-, methyl ester (8CI9CI)

GB (exp) : 172.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.3+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H3F3O2	CAS REGN : 32042-38-9

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   F
   *
   *
F**C**C**O**C++O
   *
   *
   F
```

Ethanol, 2,2,2-trifluoro-, formate (9CI)

GB (exp) : 173+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.8+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H3N	CAS REGN : 107-13-1
C++C**C##N	
2-Propenenitrile (9CI) Acrylonitrile (8CI)	
GB (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 188.3+/-2.5 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to C3H6O2(1,3-Dioxolane) with its PA value = 189.8; relative to Et CHO and MeCN	

C3H4	CAS REGN : 74-99-7
C##C**C	
1-Propyne (9CI) Propyne (8CI)	
PA (exp) : 176+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Davidson, W. R., and Bowers, M. T., Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and Cyclopropyl Cations in Gas-Phase Proton-Transfer Reactions, J. Am. Chem. Soc. 98, 6700 (1976).	
Method used : ICR Entropy change assumed zero Equilibrium; scale based on H2S.	

C3H4	CAS REGN : 463-49-0
C++C++C	
1,2-Propadiene (9CI) Allene (8CI)	
PA (exp) : 176+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Davidson, W. R., and Bowers, M. T., Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and Cyclopropyl Cations in Gas-Phase Proton-Transfer Reactions, J. Am. Chem. Soc. 98, 6700 (1976).	
Method used : ICR Equilibrium; scale based on H2S. Entropy change assumed zero.	

C3H4	CAS REGN : 2781-85-3

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   C
  * +
 *   +
C*****C
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Cyclopropene (8CI9CI)

PA (exp) : 194+/-3 kcal/mol	Temperature : 300 K

Aue, D. H., Davidson, W. R., and Bowers, M. T.,
Heats of Formation of C3H5+ Ions. Allyl, Vinyl, and
Cyclopropyl Cations in Gas-Phase Proton-Transfer Reactions,
J. Am. Chem. Soc. 98, 6700 (1976).

Method used : ICR
Bracketing relative to (CH3)2O and (C2H5)2O.

C3H4ClN	CAS REGN : 542-76-7
N##C**C**C**CL	
Propanenitrile, 3-chloro- (9CI) Propionitrile, 3-chloro- (8CI)	
PA (exp) : 181.1+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to MeCN	
GB (exp) : 178.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 186.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H5N	CAS REGN : 107-12-0
C**C**C##N	
Propanenitrile (9CI) Propionitrile (8CI)	
GB (exp) : 182.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.2+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
PA (exp) : 190.2+/-2.5 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to n-PrCN, HCO2Et, i-PrCHO, Me2O, EtCHO and relative to 1,3-Dioxane using its PA = 189.8	

C3H5N	CAS REGN : 2450-71-7
C##C**C**N	
2-Propyn-1-amine (9CI) 2-Propynylamine (8CI)	
GB (exp) : 200.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6	CAS REGN : 75-19-4

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   C
  * *
 *   *
C*****C
```

Cyclopropane (8CI9CI)

PA (exp) : 180.6+/-4 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Heats of Formation of Protonated Cyclopropane,
Methylcyclopropane, and Ethane,
J. Am. Chem. Soc. 94, 6347 (1972).

Method used : MS
HC(OH)2+ + C-C3H6 -> HCOOH + C-C3H7+.
Equilibrium of reactions:
CH3OH2+ + C-C3H6 -> CH3OH+C-C3H7+;
Apply correction for path degeneracy. Assuming
delta S=0.

C3H6	CAS REGN : 115-07-1
C++C**C	
1-Propene (9CI) Propene (8CI)	
PA (exp) : 180 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C3H7+.	
PA (exp) : 182.2+/-2 kcal/mol	Temperature : 340 K
Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).	
Method used : MS Correction for path degeneracy. Equilibrium relative to CH3OH; assuming delta S = 0.	

Continued on next page

GB (exp) : 165.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.6+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C3H6F3N	CAS REGN : 460-39-9

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          F
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          *
N**C**C**C**F
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          *
          F
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1-Propanamine, 3,3,3-trifluoro- (9CI)
Propylamine, 3,3,3-trifluoro- (8CI)

GB (exp) : 200.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H6F3N	CAS REGN : 677-41-8

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   F  C
   *  *
   *  *
F**C**N**C
   *
   *
   F
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Methanamine, 1,1,1-trifluoro-N,N-dimethyl-

PA (exp) : 192+/-3 kcal/mol	Temperature : 300 K

Staley, R. H., Taagepera, M., Henderson, W. G., Koppel, I., Beauchamp, J. L., and Taft, R. W. Effects of Alkyl and Fluoroalkyl Substitution on the Heterolytic and Homolytic Bond Dissociation Energies of Protonated Amines, J. Am. Chem. Soc. 99, 326 (1977).

Method used : ICR
Calculated entropy
Equilibrium scale based on NH3

C3H6F3N	CAS REGN : 2730-67-8

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         F
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         *
C**N**C**C**F
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         *
         F
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Ethanamine, 2,2,2-trifluoro-N-methyl- (9CI)
Ethylamine, 2,2,2-trifluoro-N-methyl- (8CI)

GB (exp) : 199.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 207.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H6N2	CAS REGN : 151-18-8
N##C**C**C**N	
Propanenitrile, 3-amino- (9CI) Propionitrile, 3-amino- (8CI)	
GB (exp) : 196.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6N2	CAS REGN : 5616-32-0
C**N**C**C##N	
Acetonitrile, (methylamino)- (8CI9CI)	
GB (exp) : 196.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6O	CAS REGN : 67-64-1
C**C**C + + O	
2-Propanone (9CI) Acetone (8CI)	
PA (exp) : 195.7+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (C2H5)2O and CH2CO	
PA (exp) : 193.6+/-1 kcal/mol	Temperature : 350 K
Ausloos, P., and Lias, S. G. The Proton Affinity of Ketene and the Heat of Formation of CH3CO+, Chem. Phys. Letters 51, 53 (1977).	
Method used : ICR Equilibrium; scale based on PA (iso-C4H8) = 193.5+/-1	

Continued on next page

GB not calculated for this reference	
PA (exp) : 188 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Delta H estimated equal 5 times translational energy of the products.	
PA (exp) : 196 kcal/mol	Temperature : 298 K
Heats of Formation of Some Isomeric [CnH2n + 1O]+ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).	
Method used : EM Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7 Lossing, F. P.	

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GB (exp) : 179+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 193.8+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 186.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 193.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H6O	CAS REGN : 123-38-6
C**C**C++O	
Propanal (9CI) Propionaldehyde (8CI)	
PA (exp) : 190+/-3 kcal/mol	Temperature :
Harrison, A. G., Ivko, A., and Van Raalte, D., Energetics of Formation of Some Oxygenated Ions and the Proton Affinities of Carbonyl Compounds, Can. J. Chem. 44, 1625 (1966).	
Method used : EI Electron impact fragmentation of various molecules.	
PA (exp) : 187 kcal/mol	Temperature : 298 K
Lossing, F. P. Heats of Formation of Some Isomeric [CnH2n + 1O]+ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).	
Method used : EM Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7	

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GB (exp) : 172.3+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 187.9+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 180.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H6O	CAS REGN : 503-30-0

```
C**O
*  *
*  *
C**C
```

Oxetane (9CI)
Trimethylene oxide (8CI)

PA (exp) : 194+/-1 kcal/mol	Temperature : 300 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Proton Affinities, Ionization Potentials, and
Hydrogen Affinities of Nitrogen and Oxygen Bases.
Hybridization Effects,
J. Am. Chem. Soc. 97, 4137 (1975).

Method used : ICR
Semiquantitative. Absolute value assign
relative to CH3CHO and (CH3)2C=CH2.

C3H6OS	CAS REGN : 1534-08-3

```
C**C**S**C
   +
   +
   O
```

Ethanethioic acid, S-methyl ester (9CI)
Acetic acid, thio-, S-methyl ester (8CI)

PA (exp) : ~197+/-2 kcal/mol	Temperature : 300 K

Grunwell, J. R., Foerst, D. L., Kaplan, F., and Siddiqui, J.
The Relative Basicity of Sulfur containing Esters, Tetrahedron 33, 2781 (1977).

Method used : ICR
Bracketing relative to MeCOOMe and MeCONHCH3. Also found the reactions of Me2S with MeCOOMe and MeCOSMe are both thermoneutral concluded PA (CH3COSCH3) is within 2 kcal of that of PA (MeCOOMe)

C3H6O2	CAS REGN : 79-09-4

```
O%%C**C**C
   %
   %
   O
```

Propanoic acid (9CI)
Propionic acid (8CI)

GB (exp) : 173.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 191.1+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C3H6O2	CAS REGN : 79-20-9
C**C**O**C + + O	
Acetic acid, methyl ester (8CI9CI)	
PA (exp) : 194+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to ME2CO and CH2CO	
GB (exp) : 186.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 194.1+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

Continued on next page

GB (exp) : 187.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 195.4+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 179.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 195.4+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C3H6O2	CAS REGN : 109-94-4
O++C**O**C**C	
Formic acid, ethyl ester (8CI9CI)	
PA (exp) : 194+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH2CO AND I-C4H8; scale based on NH3.	
GB (exp) : 183.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 191.1+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

Continued on next page

GB (exp) : 175.6+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 191.2+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 183.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H6O3	CAS REGN : 616-38-6

```
C**O**C**O**C
      +
      +
      O
```

Carbonic acid, dimethyl ester (8CI9CI)

GB (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H6S2	CAS REGN : 2168-84-5

```
      S
      +
      +
C**S****C**C
```

Ethane(dithioic)acid, methyl ester

PA (exp) : >197+/-2 kcal/mol	Temperature : 300 K

Grunwell, J. R., Forest, D. L., Kaplan, F., and Siddigui, J.
The Relative Basicity of Sulfur Containing Esters, Tetrahedron 33, 2781 (1977).

Method used : ICR
Double resonance technique shows PA (MeCSSMe) > PA (the COSMe)

C3H7N	CAS REGN : 107-11-9
C++C**C**N	
2-Propen-1-amine (9CI) Allylamine (8CI)	
GB (exp) : 205.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H7N	CAS REGN : 503-29-7

```
C**N
*  *
*  *
C**C
```

Azetidine (8CI9CI)

GB (exp) : 211.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 212.2+/-2 kcal/mol	Temperature : 290 K
PA (exp) : 220.+/-2 kcal/mol	Temperature : 290 K

Bowers, M. T., Aue, D. H., and Webb, H. M., Equilibrium Constants for Gas-Phase Ionic Reactions. Accurate Determination of Relative Proton Affinities, J. Am. Chem. Soc. 93, 4314 (1971).

Method used : ICR
Entropy change assumed zero
Equilibrium; scale based on (CH3)3N

C3H7N	CAS REGN : 1072-44-2

```
      C
     * *
    *   *
   N*****C
  *
 *
C
```

Aziridine, 1-methyl- (8CI9CI)

PA (exp) : 219.4+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Proton Affinities, Ionization Potentials, and
Hydrogen Affinities of Nitrogen and Oxygen Bases.
Hybridization Effects,
J. Am. Chem. Soc. 97, 4137 (1975).

Method used : ICR
Equilibrium; scale based on CH3NH2

C3H7NO	CAS REGN : 68-12-2

```
C**N**C++O
   *
   *
   C
```

Formamide, N,N-dimethyl- (8CI9CI)

GB (exp) : 201.2+/-3 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-3 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C3H8	CAS REGN : 74-98-6
C**C**C	
Propane (8CI9CI)	
PA (exp) : 148.2 kcal/mol	Temperature : 163-213 K
Hiraoka, K., and Kebarle, P., Information on the Proton Affinity and Protolysis of Propane from Measurement of the Ion Cluster, Equilibrium: C2H5+ + CH4 = C3H9+. Can. J. Chem. 53, 970 (1975).	
Method used : MS Equilibrium of reaction C2H5+ + 2CH4 -> C3H9+ + CH4 Van't Hoff plot	
PA (exp) : 143 kcal/mol	Temperature : 170 K
Field, F. H., and Beggs, D. P., Reversible Reactions of Gaseous Ions. III. Studies with Methane at 0.1-1.0 Torr and 77-300 K, J. Am. Chem. Soc. 93, 1585 (1971).	
Method used : MS Equilibrium of reaction: C2H5+ + CH4 -> C3H9+. Based on delta H formation(C2H5+). Calculated entropy	

Continued on next page

GB not calculated for this reference	
PA (exp) : <152.8 kcal/mol	Temperature : ~170 K

Hiraoka, K., and Kebarle, P.,
Stabilities and Energetics of Pentacoordinated
Carbonium Ions. The Isomeric C2H7+ Ions and Some
Higher Analogues: C3H9+ and C4H11+,
J. Am. Chem. Soc. 98, 6119 (1976).

Method used : MS
Calculated entropy
Equilibrium of reaction
Sec-C3H7+ + H2 -> C3H9+
Based on delta H formation(C3H7+);
C-H protonation

C3H8O	CAS REGN : 67-63-0

```
C**C**C
   *
   *
   O
```

2-Propanol (9CI)
Isopropyl alcohol (8CI)

PA (exp) : 192+/-2 kcal/mol	Temperature : 323-373 K

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to I-C4H8 and (CH3)2O

Continued on next page

GB not calculated for this reference	
PA (exp) : 190 kcal/mol	Temperature :
Hiraoka, K., and Kebarle, P. Condensation Reactions Involving Carbonium Ions and Lewis Bases in the Gas Phase. Hydration of the tert-Butyl Cation, J. Am. Chem. Soc. 99, 360 (1977).	
Method used : MS Equilibrium relative to known standard acids	

C3H8O	CAS REGN : 71-23-8
C**C**C**O	
1-Propanol (9CI) Propyl alcohol (8CI)	
GB (exp) : 181.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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PA (exp) : 189+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to C2H5OH and (CH3)2O	

C3H8O	CAS REGN : 540-67-0
C**C**O**C	
Ethane, methoxy- (9CI) Ether, ethyl methyl (8CI)	
GB (exp) : 186.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 194+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H8S	CAS REGN : 75-33-2
C**C**C * * S	
2-Propanethiol (8CI9CI)	
GB (exp) : 184.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 192+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H8S	CAS REGN : 107-03-9
C**C**C**S	
1-Propanethiol (8CI9CI)	
GB (exp) : 181.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H8S	CAS REGN : 624-89-5
C**C**S**C	
Ethane, (methylthio)- (9CI) Sulfide, ethyl methyl (8CI)	
GB (exp) : 192.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C3H9As	CAS REGN : 593-88-4
C**AS*C * * C	
Arsine, trimethyl- (8CI9CI)	
PA (exp) : 210.6 kcal/mol	Temperature : 300 K
Hodges, R. V., and Beauchamp, J. L., Basicity and Ion-Molecule Reactions of Trimethylarsine in the Gas Phase Determined by Ion Cyclotron Resonance Spectroscopy, Inorg. Chem. 14, 2887 (1975).	
Method used : ICR Equilibrium relative to CH3NH2 and also to CF3(CH2)3NH2.	

C3H9N	CAS REGN : 75-31-0
C**C**C * * N	
2-Propanamine (9CI) Isopropylamine (8CI)	
GB (exp) : 208.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 216.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 208.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.6+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C3H9N	CAS REGN : 75-50-3
C**N**C * * C	
Methanamine, N,N-dimethyl- (9CI) Trimethylamine (8CI)	
GB (exp) : 214.30+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 222.10+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 213.70+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 221.50+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

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GB (exp) : 208.40+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 225.60+/-2 kcal/mol	Temperature : 600 K

Briggs, J. P., Yamdagni, R., and Kebarle, P.,
Intrinsic Basicities of Ammonia, Methylamines,
Anilines, and Pyridine from Gas-Phase Proton-
Exchange Equilibria,
J. Am. Chem. Soc. 94, 5128 (1972).

Method used : MS
Entropy change assumed zero
Equilibrium; scale based on NH3

C3H9N	CAS REGN : 107-10-8

C**C**C**N

1-Propanamine (9CI)
Propylamine (8CI)

GB (exp) : 207.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 215.5+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 207.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 215.7+/-2 kcal/mol	Temperature : 300 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C3H9N	CAS REGN : 624-78-2
C**C**N**C	
Ethanamine, N-methyl- (9CI) Ethylamine, N-methyl- (8CI)	
GB (exp) : 212.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

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GB (exp) : 212+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 220.2+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C3H9NO	CAS REGN : 109-85-3

C**O**C**C**N

Ethanamine, 2-methoxy- (9CI)
Ethylamine, 2-methoxy- (8CI)

GB (exp) : 209.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 221.0+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Evaluation of Intramolecular Strong
Hydrogen Bonding in the Gas Phase,
J. Am. Chem. Soc. 95, 2669 (1973).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C3H9P	CAS REGN : 594-09-2
C**P**C * * C	
Phosphine, trimethyl- (8CI9CI)	
GB (exp) : 214.9+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	
PA (exp) : 223.3+/-2 kcal/mol	Temperature : 300 K
Staley, P. H., and Beauchamp, J. L. Basicities and Ion-Molecule Reactions of the Methylphosphines in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 96, 6252 (1974).	
Method used : ICR Bracketing relative to (CH3)3N and (CH3)2C2H5N	

C3H10N2	CAS REGN : 109-76-2
N**C**C**C**N	
1,3-Propanediamine (8CI9CI)	
GB (exp) : 219.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 231.60+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 221.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.10+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

C4H4F4O2	CAS REGN : 1683-88-1

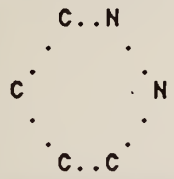
```
   F
   *
   *
F**C**C**O**C**C**F
   *  +
   *  +
   F  O
```

Acetic acid, trifluoro-, 2-fluoroethyl ester (8CI)

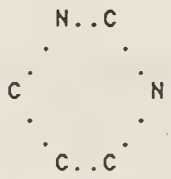
GB (exp) : 172.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H4N2	CAS REGN : 289-80-5
	
Pyridazine (8CI9CI)	
GB (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H4N2	CAS REGN : 289-95-2



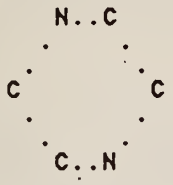
Pyrimidine (8CI9CI)

GB (exp) : 201.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H4N2	CAS REGN : 290-37-9



Pyrazine (8CI9CI)

GB (exp) : 199.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H4N2O	CAS REGN : 557-01-7

```
      C
     . .
    .   .
   N     C
   .     .
   .     .
O%%C     C
    .   .
     . .
      N
```

2(1H)-Pyrimidinone (8CI9CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C4H4N2O2	CAS REGN : 66-22-8

```
      C
     . .
    .   .
   C     N
   .     .
   .     .
O%%C     C%%O
    .   .
     . .
      N
```

2,4(1H,3H)-Pyrimidinedione (9CI)
Uracil (8CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C4H4O	CAS REGN : 110-00-9

```
C*****O
+     *
+     *
C     C
 *   +
  * +
   C
```

Furan (8CI9CI)

PA (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K

Chong, S. L., and Franklin, J. L.,
Proton Affinities of Benzene, Toluene, and the Xylenes,
J. Am. Chem. Soc. 94, 6630 (1972).

Method used : MS
Entropy change assumed zero
Equilibrium relative to (CH3)2O.

C4H5F3O2	CAS REGN : 383-63-1

```
   F
   *
   *
F**C**C**O**C**C
   *  +
   *  +
   F  O
```

Acetic acid, trifluoro-, ethyl ester (8CI9CI)

GB (exp) : 175.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 183.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H5N	CAS REGN : 109-97-7

```
C*****N
+     *
+     *
C     C
 *   +
  * +
   C
```

1H-Pyrrole (9CI)
Pyrrole (8CI)

GB (exp) : 197.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 205.9+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

GB (exp) : 192.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 209.4+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C4H5N	CAS REGN : 5500-21-0

```
        C
       * *
      *   *
     C*****C
    *
   *
N##C
```

Cyclopropanecarbonitrile (8CI9CI)

PA (exp) : 193.2+/-2 kcal/mol	Temperature : 300 K

Staley, R. H., Kleckner, J. E., and Beauchamp, J. L.
Relationship between Orbital Ionization Energies
and Molecular Properties. Proton Affinities and
Photoelectron Spectra of Nitriles,
J. Am. Chem. Soc. 98, 2081 (1976).

Method used : ICR
Calculated entropy
Equilibrium relative to HCO2-n-C4H9

GB (exp) : 185.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 193.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,
McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of
Compounds between Water and Ammonia from Pulsed Ion
Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H5NO2	CAS REGN : 623-49-4

```
N##C**C**O**C**C
      +
      +
      O
```

Carbonocyanidic acid, ethyl ester (9CI)
Formic acid, cyano-, ethyl ester (8CI)

GB (exp) : 173.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H5N3O	CAS REGN : 71-30-7

```
      C
     . .
    .   .
   C     N
   .     .
   .     .
N%%C     C%%O
    .   .
     . .
      N
```

2(1H)-Pyrimidinone, 4-amino- (9CI)
Cytosine (8CI)

PA (exp) : 220+/-2 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)2NH and (CH3)3N.

C4H6N2	CAS REGN : 616-47-7

```
   C+++++N
   *     *
   *     *
C**N     C
    *   +
     * +
      C
```

1H-Imidazole, 1-methyl- (9CI)
Imidazole, 1-methyl- (8CI)

GB (exp) : 217.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 225.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H7F3O	CAS REGN : 461-24-5

```
   F
   *
   *
F**C**C**O**C**C
   *
   *
   F
```

Ethane, 2-ethoxy-1,1,1-trifluoro- (9CI)
Ether, ethyl 2,2,2-trifluoroethyl (8CI)

GB (exp) : 177.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 184.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H7N	CAS REGN : 78-82-0

```
C**C**C##N
   *
   *
   C
```

Propanenitrile, 2-methyl- (9CI)
Isobutyronitrile (8CI)

PA (exp) : 192.2+/-2 kcal/mol	Temperature : 300 K

Staley, R. H., Kleckner, J. E., and Beauchamp, J. L.
Relationship between Orbital Ionization Energies
and Molecular Properties. Proton Affinities and
Photoelectron Spectra of Nitriles,
J. Am. Chem. Soc. 98, 2081 (1976).

Method used : ICR
Calculated entropy
Equilibrium relative to HCO2C2H5

GB (exp) : 184.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 192.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,
McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of
Compounds between Water and Ammonia from Pulsed Ion
Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H7N	CAS REGN : 109-74-0
N##C**C**C**C	
Butanenitrile (9CI) Butyronitrile (8CI)	
PA (exp) : 191.2+/-2.5 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to HCO2Et, ME2O and EtCN	
GB (exp) : 183.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.4+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8	CAS REGN : 106-98-9
C**C**C++C	
1-Butene (8CI9CI)	
PA (exp) : 183.2 kcal/mol	Temperature : 298 K

Lossing F. P., and Semeluk, G. P.
Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals,
Can. J. Chem. 48, 955 (1970).

Method used : EM
Appearance potential of C4H9+ by EM

C4H8	CAS REGN : 115-11-7

```
C**C**C
   +
   +
   C
```

1-Propene, 2-methyl- (9CI)
Propene, 2-methyl- (8CI)

PA (exp) : 192.6+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Using delta Hf(t-C4H9+) = 169+/-1.8 derived from,
delta Hf(t-C4H9) = 9.3 and IP(t-C4H9) = 159.9

PA (exp) : 193.7 kcal/mol	Temperature :

Lossing F. P., and Semeluk, G. P.
Free Radicals by Mass Spectrometry. XLII. Ionization
Potentials and Ionic Heats of Formation for C1-C4
Alkyl Radicals,
Can. J. Chem. 48, 955 (1970).

Method used : EM
Appearance potential of C4H9+

Continued on next page

GB (exp) : 177.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 194.2+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 185.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 193.5+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8	CAS REGN : 590-18-1
C**C++C**C	
2-Butene, (Z)- (8CI9CI)	
PA (exp) : 181.9 kcal/mol	Temperature : 298 K

Lossing F. P., and Semeluk, G. P.
Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals,
Can. J. Chem. 48, 955 (1970).

Method used : EM
Appearance potential of C4H9+

C4H8	CAS REGN : 594-11-6

```
      C
     * *
    *   *
   C*****C
  *
 *
C
```

Cyclopropane, methyl- (8CI9CI)

PA (exp) : 181+/-2 kcal/mol	Temperature :

Chong, S. L., and Franklin, J. L.,
Heats of Formation of Protonated Cyclopropane,
Methylcyclopropane, and Ethane,
J. Am. Chem. Soc. 94, 6347 (1972).

Method used : MS
Equilibrium relative to HCOOH
based on PA(HCOOH)=180.1+/-2 assuming delta S=0
Correction for path degeneracy.

C4H8	CAS REGN : 624-64-6
C**C++C**C	
2-Butene, (E)- (8CI9CI)	
PA (exp) : 180.9 kcal/mol	Temperature : 298 K
Lossing F. P., and Semeluk, G. P. Free Radicals by Mass Spectrometry. XLII. Ionization Potentials and Ionic Heats of Formation for C1-C4 Alkyl Radicals, Can. J. Chem. 48, 955 (1970).	
Method used : EM Appearance potential of C4H9+	

C4H8F3N	CAS REGN : 819-06-7

```
          F
          *
          *
C**N**C**C**F
   *      *
   *      *
   C      F
```

Ethanamine, 2,2,2-trifluoro-N,N-dimethyl- (9CI)
Ethylamine, 2,2,2-trifluoro-N,N-dimethyl- (8CI)

GB (exp) : 204.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H8F3N	CAS REGN : 819-46-5

```
   F
   *
   *
F**C**C**C**C**N
   *
   *
   F
```

1-Butanamine, 4,4,4-trifluoro- (9CI)
Butylamine, 4,4,4-trifluoro- (8CI)

GB (exp) : 203.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H8N2	CAS REGN : 926-64-7
N##C**C**N**C * * C	
Acetonitrile, (dimethylamino)- (8CI9CI)	
GB (exp) : 200.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O	CAS REGN : 78-84-2

```
C**C**C++O
   *
   *
   C
```

Propanal, 2-methyl- (9CI)
Isobutyraldehyde (8CI)

GB (exp) : 182.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H8O	CAS REGN : 78-93-3

```
C**C**C**C
   +
   +
   O
```

2-Butanone (8CI9CI)

GB (exp) : 189.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 193.7+/-1 kcal/mol	Temperature : 293 K

Lossing, F. P.
Heats of Formation of Some Isomeric [CnH2n + 1O]+ Ions. Substitutional Effects on Ion Stability, J. Am. Chem. Soc. 99, 7526 (1977).

Method used : EM
Electron impact fragmentation (various molecules) using EM. delta Hf(H+) = 365.7

C4H8O	CAS REGN : 109-99-9

```
C*****O
*     *
*     *
C     C
 *   *
  * *
   C
```

Furan, tetrahydro- (8CI9CI)

GB (exp) : 189+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.4+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H8O	CAS REGN : 123-72-8
O++C**C**C**C	
Butanal (9CI) Butyraldehyde (8CI)	
GB (exp) : 181.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O2	CAS REGN : 110-74-7
C**C**C**O**C++O	
Formic acid, propyl ester (8CI9CI)	
PA (exp) : 194+/-2 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH2CO AND I-C4H8; scale based on NH3.	
GB (exp) : 184.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 192.1+/-2 kcal/mol	Temperature : 298 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

Continued on next page

GB (exp) : 184.5 kcal/mol	Temperature : 300 K
PA (exp) : 192.3+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 176.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 191.7+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C4H8O2	CAS REGN : 123-91-1

```
   O**C
  *    *
 *      *
C        C
 *      *
  *    *
   C**O
```

1,4-Dioxane (9CI)
p-Dioxane (8CI)

GB (exp) : 183.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.9+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H8O2	CAS REGN : 141-78-6

```
C**C**O**C**C
         +
         +
         O
```

Acetic acid ethyl ester (8CI9CI)

PA (exp) : 197+/-2 kcal/mol	Temperature : 323-373 K

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to (C2H5)2O and CH3CO2ME.

GB (exp) : 188.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196+/-2 kcal/mol	Temperature : 300 K

Harrison, A. G., Lin, P. H., and Tsang, C. W.,
Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,
Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).

Method used : MS
Equilibrium; scale based on (CH3)2CO
Entropy change assumed zero

Continued on next page

GB (exp) : 190.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.1+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 182.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 198+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	

C4H8O2	CAS REGN : 554-12-1

```
C**O**C**C**C
      +
      +
      O
```

Propanoic acid, methyl ester (9CI)
Propionic acid, methyl ester (8CI)

GB (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 197+/-2 kcal/mol	Temperature : 323-373 K

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to (C2H5)2O and CH3COOMe

C4H8O2	CAS REGN : 625-55-8

```
O++C**O**C**C
         *
         *
         C
```

Formic acid, 1-methylethyl ester (9CI)
Formic acid, isopropyl ester (8CI)

GB (exp) : 185.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 193.2+/-2 kcal/mol	Temperature : 298 K

Harrison, A. G., Lin, P. H., and Tsang, C. W.,
Proton Transfer Reactions by Trapped-Ion Mass Spectrometry,
Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).

Method used : MS
Equilibrium; scale based on (CH3)2CO
Entropy change assumed zero

C4H8O2S	CAS REGN : 38103-96-7
C**O**C**S**C**C + + O	
Carbonothioic acid, S-ethyl O-methyl ester (9CI)	
GB (exp) : 190.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H8O3	CAS REGN : 623-53-0

```
C**O**C**O**C**C
      +
      +
      O
```

Carbonic acid, ethyl methyl ester (8CI9CI)

GB (exp) : 192.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H9N	CAS REGN : 123-75-1

```
C*****N
*     *
*     *
C     C
 *   *
  * *
   C
```

Pyrrolidine (8CI9CI)

GB (exp) : 213.70+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.90+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 213.30+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 221.50+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C4H9N	CAS REGN : 1190-79-0
C**C++N**C**C	
Ethanamine, N-ethylidene- (9CI) Ethylamine, N-ethylidene- (8CI)	
PA (exp) : 220.5+/-2 kcal/mol	Temperature :
Aue, D. H., Webb, H. M., and Bowers, M. T., Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Nitrogen and Oxygen Bases. Hybridization Effects, J. Am. Chem. Soc. 97, 4137 (1975).	
Method used : ICR Equilibrium; scale based on CH3NH2	

C4H9NO	CAS REGN : 110-91-8

```
   O**C
  *    *
 *      *
C        C
 *      *
  *    *
   C**N
```

Morpholine (8CI9CI)

GB (exp) : 208.6+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.8+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C4H9NO	CAS REGN : 127-19-5
C**C**N**C + * + * O C	
Acetamide, N,N-dimethyl- (8CI9CI)	
GB (exp) : 205.4+/-2.5 kcal/mol	Temperature : 300 K
Taft, R. W., Proton-Transfer Reactions, Ed. E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	

C4H9NO	CAS REGN : 563-83-7
C**C**C%%N * % * % C O	
Propanamide, 2-methyl- (9CI) Isobutyramide (8CI)	
GB (exp) : 206.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.9+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H10	CAS REGN : 106-97-8
C**C**C**C	
Butane (8CI9CI)	
PA (exp) : 166.8 (2) kcal/mol	Temperature : 291 K
Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C2H7+ Ions and Some Higher Analogues: C3H9+ and C4H11+, J. Am. Chem. Soc. 98, 6119 (1976).	
Method used : MS Van't Hoff plot C-H protonation (2) Equilibrium of reaction t-C4H9+ + H2 -> C4H11+ (2)	
PA (exp) : 164 (1) kcal/mol	Temperature : 291 K
Hiraoka, K., and Kebarle, P., Stabilities and Energetics of Pentacoordinated Carbonium Ions. The Isomeric C2H7+ Ions and Some Higher Analogues: C3H9+ and C4H11+, J. Am. Chem. Soc. 98, 6119 (1976).	
Method used : MS Van't Hoff plot C-C protonation (1) Equilibrium of reaction C3H7+ + CH4 -> C4H11+ (1)	

C4H10N2	CAS REGN : 110-85-0

```
   N**C
  *    *
 *      *
C        C
 *      *
  *    *
   C**N
```

Piperazine (8CI9CI)

GB (exp) : 210.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 218.9+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C4H10O	CAS REGN : 60-29-7
C**C**O**C**C	
Ethane, 1,1'-oxybis- (9CI) Ethyl ether (8CI)	
PA (exp) : 198+/-4 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to (CH3)2CO and NH3.	
GB (exp) : 188.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.1+/-2 kcal/mol	Temperature : 300 K
Harrison, A. G., Lin, P. H., and Tsang, C. W., Proton Transfer Reactions by Trapped-Ion Mass Spectrometry, Int. J. Mass Spectrom. Ion Phys. 19, 23 (1976).	
Method used : MS Equilibrium; scale based on (CH3)2CO Entropy change assumed zero	

Continued on next page

GB (exp) : 182.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 197.3+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 190+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.4+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H10O	CAS REGN : 71-36-3
O**C**C**C**C	
1-Butanol (9CI) Butyl alcohol (8CI)	
GB (exp) : 181.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H10O	CAS REGN : 75-65-0

```
   O
   *
   *
C**C**C
   *
   *
   C
```

2-Propanol, 2-methyl- (9CI)
tert-Butyl alcohol (8CI)

PA (exp) : 194+/-1 kcal/mol	Temperature :

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to CH2CO and I-C5H10

PA (exp) : 192 kcal/mol	Temperature :

Hiraoka, K., and Kebarle, P.
Condensation Reactions Involving Carbonium Ions and Lewis Bases in the Gas Phase. Hydration of the tert-Butyl Cation,
J. Am. Chem. Soc. 99, 360 (1977).

Method used : MS
Equilibrium relative to known standard acids

C4H10S	CAS REGN : 75-66-1

```
   S
   *
   *
C**C**C
   *
   *
   C
```

2-Propanethiol, 2-methyl- (8CI9CI)

GB (exp) : 186.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C4H10S	CAS REGN : 352-93-2
C**C**S**C**C	
Ethane, 1,1'-thiobis- (9CI) Ethyl sulfide (8CI)	
GB (exp) : 195.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 202.6+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C4H11N	CAS REGN : 75-64-9

```
   N
   *
   *
C**C**C
   *
   *
   C
```

2-Propanamine, 2-methyl- (9CI)
tert-Butylamine (8CI)

GB (exp) : 210.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 218.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 210.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 218.6+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on CH3NH2

C4H11N	CAS REGN : 78-81-9
C**C**C**N * * C	
1-Propanamine, 2-methyl- (9CI) Isobutylamine (8CI)	
GB (exp) : 207.7+/-2 kcal/mol	Temperature : 298 K
Taft, R. W., Proton-Transfer Reactions, Ed, E. F. Caldin and V. Gold, (John Wiley and Sons, New York, 1975) Ch. 2.	
Method used : ICR Equilibrium; scale based on NH3	
GB (exp) : 208.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.7+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 109-73-9
N**C**C**C**C	
1-Butanamine (9CI) Butylamine (8CI)	
GB (exp) : 207.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 216+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 207.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.2+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects, J. Am. Chem. Soc. 98, 318 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 109-89-7
C**C**N**C**C	
Ethanamine, N-ethyl- (9CI) Diethylamine (8CI)	
GB (exp) : 214.50+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 222.70+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 214.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 222.30+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potontials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 598-56-1
C**N**C**C * * C	
Ethanamine, N,N-dimethyl- (9CI) Ethylamine, N,N-dimethyl- (8CI)	
GB (exp) : 216.70+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.50+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 216.00+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 223.80+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C4H11N	CAS REGN : 13952-84-6

```
C**C**C**C
   *
   *
   N
```

2-Butanamine (9CI)
sec-Butylamine (8CI)

GB (exp) : 208.9 kcal/mol	Temperature : 300 K

Taft, R. W.,
Proton-Transfer Reactions,
Ed. E. F. Caldin and V. Gold,
(John Wiley and Sons, New York, 1975) Ch. 2.

Method used : ICR
Equilibrium; scale based on NH3

GB (exp) : 209.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.7+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C4H12N2	CAS REGN : 110-60-1
N**C**C**C**C**N	
1,4-Butanediamine (8CI9CI)	
GB (exp) : 221.70+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 236.60+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5Fe05	CAS REGN : 13463-40-6

```
       O
       #
       #
       C   C##O
       * *
       **
O##C**FE*C##O
       *
       *
       C
       #
       #
       O
```

Iron carbonyl (Fe(CO)5), (TB-5-11)- (9CI)
Iron carbonyl (Fe(CO)5) (8CI)

PA (exp) : 200+/-3 kcal/mol	Temperature : 300 K

Foster, M. S., and Beauchamp, J. L.,
Gas-Phase Ion Chemistry of Iron Pentacarbonyl by
Ion Cyclotron Resonance Spectroscopy. New Insights
into the Properties and Reactions of Transition
Metal Complexes in the Absence of Complicating
Solvation Phenomena,
J. Am. Chem. Soc. 97, 4808 (1975).

Method used : ICR
Bracketing relative to (CH3O)2CO and NH3.

C5H3ClN4	CAS REGN : 87-42-3

```
       C
      . .
     .   .
    N     N
    .     .
    .     .
CL*C      C
     .   . %
      . .   %
       C     N
       *     %
       *     %
       N%%%%%C
```

1H-Purine, 6-chloro- (9CI)
Purine, 6-chloro- (8CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C5H4ClN	CAS REGN : 109-09-1

```
      C
     . .
    .   .
   N     C
   .     .
   .     .
CL*C     C
    .   .
     . .
      C
```

Pyridine, 2-chloro- (8CI9CI)	
GB (exp) : 204.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H4ClN	CAS REGN : 626-60-8

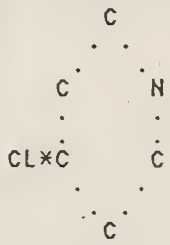
```
      N
     . .
    .   .
   C     C
   .     .
   .     .
CL*C     C
    .   .
     . .
      C
```

Pyridine, 3-chloro- (8CI9CI)

GB (exp) : 204.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H4ClN	CAS REGN : 626-61-9
	
Pyridine, 4-chloro- (8CI9CI)	
GB (exp) : 207.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 215+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H4FN	CAS REGN : 372-47-4

```
      N
     . .
    .   .
   C     C
   .     .
   .     .
F**C     C
    .   .
     . .
      C
```

Pyridine, 3-fluoro- (8CI9CI)

GB (exp) : 203.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.5+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H4FN	CAS REGN : 372-48-5

```
      C
     . .
    .   .
   N     C
   .     .
   .     .
F**C     C
    .   .
     . .
      C
```

Pyridine, 2-fluoro- (8CI9CI)

GB (exp) : 200.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H4FN	CAS REGN : 694-52-0

```
      C
     . .
    .   .
   C     N
   .     .
   .     .
F**C     C
    .   .
     . .
      C
```

Pyridine, 4-fluoro- (8CI9CI)

GB (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H4N2O2	CAS REGN : 1122-61-8

```
          C
         . .
        .   .
       C     N
       .     .
       .     .
O++N**C      C
   +   .   .
   +    . .
   O     C
```

Pyridine, 4-nitro- (8CI9CI)

GB (exp) : 198.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 201+/-2 kcal/mol	Temperature : 300 K

Taagepera, M., Henderson, W. G., Brownlee, R. T. C., Beauchamp, J. L., Holtz, D., and Taft, R. W., Gas-Phase Basicities and Pyridine Substituent Effects. J. Am. Chem. Soc. 94, 1369 (1972).

Method used : ICR
Equilibrium; scale based on Pyridine

C5H4N4O	CAS REGN : 68-94-0

```
       C
      . .
     .   .
   N       N
   .       .
   .       .
O%%C       C
     .    . %
      .  .   %
       C      N
       *      %
       *      %
       N%%%%%C
```

6H-Purin-6-one, 1,7-dihydro- (9CI)
Hypoxanthine (8CI)

PA (exp) : 215+/-4 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to CH3NH2 and (CH3)2NH.

C5H5N	CAS REGN : 110-86-1

```
   C..N
  .    .
 .      .
C        C
 .      .
  .    .
   C..C
```

Pyridine (8CI9CI)

GB (exp) : 210.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 218.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to (CH3)2NH

Continued on next page

GB (exp) : 209.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.6+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

GB (exp) : 203.7+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 220.9+/-2 kcal/mol	Temperature : 600 K

Briggs, J. P., Yamdagni, R., and Kebarle, P.,
Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phas Proton-Exchange Equilibria,
J. Am. Chem. Soc. 94, 5128 (1972).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C5H5N5	CAS REGN : 73-24-5

```
       C
      . .
     .   .
    N     N
    .     .
    .     .
N%%C      C
     .   . %
      . .   %
       C     N
       *     %
       *     %
       N%%%%%C
```

1H-Purin-6-amine (9CI)
Adenine (8CI)

PA (exp) : 220+/-2 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)2NH and (CH3)3N

C5H5N5O	CAS REGN : 73-40-5

```
C%%N
%   %
%    %
%     C..N
%    .    .
%   .      .
N**C        C%%N
     :      .
      .    .
       C..N
       %
       %
       O
```

6H-Purin-6-one, 2-amino-1,7-dihydro- (9CI)
Guanine (8CI)

PA (exp) : 220+/-2 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)2NH and (CH3)3N.

C5H6N2O2	CAS REGN : 65-71-4

```
      C..N
     .    .
    .      .
C**C        C%%O
    .      .
     .    .
      C..N
      %
      %
      O
```

2,4(1H,3H)-Pyrimidinedione, 5-methyl- (9CI)
Thymine (8CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2

C5H7F3O2	CAS REGN : 383-66-4

```
   F
   *
   *
F**C**C**O**C**C**C
   *  +
   *  +
   F  O
```

Acetic acid, trifluoro-, propyl ester (8CI9CI)

GB (exp) : 176.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 184.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H8	CAS REGN : 693-86-7

```
        C
       * *
      *   *
     C*****C
    *
   *
C++C
```

Cyclopropane, ethenyl- (9CI)
Cyclopropane, vinyl- (8CI)

GB (exp) : 187.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 195.2+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H8O	CAS REGN : 765-43-5

```
        C
       * *
      *   *
     C*****C
    *
   *
C**C
   +
   +
   O
```

Ethanone, 1-cyclopropyl- (9CI)
Ketone, cyclopropyl methyl (8CI)

GB (exp) : 194.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 202.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H8O2	CAS REGN : 123-54-6

```
C**C**C**C**C
   +     +
   +     +
   O     O
```

2,4-Pentanedione (8CI9CI)

GB (exp) : 197.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.6+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia From Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H8O2	CAS REGN : 2868-37-3

```
            C
           * *
          *   *
        C*****C
       *
      *
C**O**C
      +
      +
      O
```

Cyclopropanecarboxylic acid, methyl ester (8CI9CI)

GB (exp) : 192.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H9N	CAS REGN : 110-59-8
C**C**C**C**C##N	
Pentanenitrile (9CI) Valeronitrile (8CI)	
PA (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Kleckner, J. E., and Beauchamp, J. L. Relationship between Orbital Ionization Energies and Molecular Properties. Proton Affinities and Photoelectron Spectra of Nitriles, J. Am. Chem. Soc. 98, 2081 (1976).	
Method used : ICR Calculated entropy Equilibrium relative to HCO2C2H5	
GB (exp) : 184.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H10	CAS REGN : 513-35-9

```
C**C++C**C
   *
   *
   C
```

2-Butene, 2-methyl- (8CI9CI)

PA (exp) : 194.4+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Van't Hoff plot
Equilibrium of hydride transfer reaction between (t-C4H9+) + Me2CHEt. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169

C5H10	CAS REGN : 563-46-2

```
C**C**C**C
   +
   +
   C
```

1-Butene, 2-methyl- (8CI9CI)

PA (exp) : 193.5+/-2 kcal/mol	Temperature :

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to Iso-C4H8

PA (exp) : 197.32 kcal/mol	Temperature : 300 K

Solomon, J. J., and Field, F. H.,
Reversible Reactions of Gaseous Ions. IX. The
Stability of C4-C7 Tertiary Alkyl Carbonium Ions,
J. Am. Chem. Soc. 97, 2625 (1975).

Method used : MS
Equilibrium scale Based on delta H formation(T-C4H9+)
= 169 Kcal/mol.

Continued on next page

GB not calculated for this reference	
PA (exp) : 195.9+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Equilibrium of hydride transfer reaction between (t-C4H9+) + Me2CHEt. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169

C5H10O	CAS REGN : 96-22-0

```
C**C**C**C**C
      +
      +
      O
```

3-Pentanone (8CI9CI)

GB (exp) : 191.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.5+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H10O	CAS REGN : 96-47-9

```
   O*****C
   *     *
   *     *
C**C     C
    *   *
     * *
      C
```

Furan, tetrahydro-2-methyl- (8CI9CI)

GB (exp) : 192.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H10O	CAS REGN : 110-62-3
C**C**C**C**C++O	
Pentanal (9CI) Valeraldehyde (8CI)	
GB (exp) : 182.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H10O	CAS REGN : 142-68-7

```
   C**O
  *    *
 *      *
C        C
 *      *
  *    *
   C**C
```

2H-Pyran, tetrahydro- (8CI9CI)

GB (exp) : 189.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.1+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H10O	CAS REGN : 563-80-4

```
C**C**C**C
   *  +
   *  +
   C  O
```

2-Butanone, 3-methyl- (8CI9CI)

GB (exp) : 190.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H10O2	CAS REGN : 109-60-4

```
C**C**O**C**C**C
   +
   +
   O
```

Acetic acid, propyl ester (8CI9CI)

PA (exp) : 200+/-3 kcal/mol	Temperature :

Long, J., and Munson, B.,
Proton Affinities of Some Oxygenated Compounds,
J. Am. Chem. Soc. 95, 2427 (1973).

Method used : MS
Bracketing relative to NH3 and CH3COOC2H5.

GB (exp) : 182.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 200.1+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds
Between Water and Ammonia and Substituted Benzenes from
A Continuous Ladder of Proton Transfer Equilibria
Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C5H10O2	CAS REGN : 547-63-7

```
C**O**C**C**C
      +  *
      +  *
      O  C
```

Propanoic acid, 2-methyl-, methyl ester (9CI)
Isobutyric acid, methyl ester (8CI)

GB (exp) : 191.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H10O2	CAS REGN : 592-84-7
O++C**O**C**C**C**C	
Formic acid, butyl ester (8CI9CI)	
GB (exp) : 184.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 192.5+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H11N	CAS REGN : 110-89-4

```
   C**N
  *    *
 *      *
C        C
 *      *
  *    *
   C**C
```

Piperidine (8CI9CI)

GB (exp) : 214.90+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 223.10+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 214.40+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 222.60+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

Continued on next page

GB (exp) : 209.60+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 226.80+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding
in Proton-Bound Amine Dimers and Proton-Induced
Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C5H11N	CAS REGN : 120-94-5

```
   C*****C
   *     *
   *     *
C**N     C
    *   *
     * *
      C
```

Pyrrolidine, 1-methyl- (8CI9CI)

GB (exp) : 217.80+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 225.60+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 217.30+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.10+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C5H11NO2	CAS REGN : 687-48-9

```
C**N**C**O**C**C
   *  +
   *  +
   C  O
```

Carbamic acid, dimethyl-, ethyl ester (8CI9CI)

GB (exp) : 203.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H12O	CAS REGN : 625-54-7

```
C**C**O**C**C
          *
          *
          C
```

Propane, 2-ethoxy- (9CI)
Ether, ethyl isopropyl (8CI)

GB (exp) : 192.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.7+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H12O	CAS REGN : 1634-04-4

```
   C
   *
   *
C**C**O**C
   *
   *
   C
```

Propane, 2-methoxy-2-methyl- (9CI)
Ether, tert-butyl methyl (8CI)

GB (exp) : 191.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.5+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C5H13N	CAS REGN : 110-58-7
C**C**C**C**C**N	
1-Pentanamine (9CI) Pentylamine (8CI)	
GB (exp) : 208+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.4+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5H13N	CAS REGN : 594-39-8

```
   N
   *
   *
C**C**C**C
   *
   *
   C
```

2-Butanamine, 2-methyl- (9CI)
tert-Pentylamine (8CI)

GB (exp) : 211.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 211.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 219.5+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C5H13N	CAS REGN : 616-39-7
C**C**N**C**C * * C	
Ethanamine, N-ethyl-N-methyl- (9CI) Diethylamine, N-methyl- (8CI)	
GB (exp) : 218.90+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.70+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 218.40+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 226.20+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C5H13N	CAS REGN : 996-35-0
C**C**N**C * * * * C C	
2-Propanamine, N,N-dimethyl- (9CI) Ethylamine, N,N,1-trimethyl- (8CI)	
GB (exp) : 218.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.7+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H13N	CAS REGN : 5813-64-9

```
   C
   *
   *
C**C**C**N
   *
   *
   C
```

1-Propanamine, 2,2-dimethyl- (9CI)
Neopentylamine (8CI)

GB (exp) : 208.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 209.0+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 217.4+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C5H13N	CAS REGN : 19961-27-4
C**C**N**C**C * * C	
2-Propanamine, N-ethyl- (9CI) Diethylamine, 1-methyl- (8CI)	
GB (exp) : 216+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.2+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C5H14N2	CAS REGN : 109-55-7
C**N**C**C**C**N * * C	
1,3-Propanediamine, N,N-dimethyl- (8CI9CI)	
GB (exp) : 225.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Equilibrium; scale based on NH3	

C5H14N2	CAS REGN : 462-94-2
N**C**C**C**C**C**N	
1,5-Pentanediamine (8CI9CI)	
GB (exp) : 220.00+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 234.60+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 221.40+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.10+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

C6F6	CAS REGN : 392-56-3

```
      F   F
      *   *
      *   *
      C..C
     .     .
    .       .
F**C         C**F
    .       .
     .     .
      C..C
      *   *
      *   *
      F   F
```

Benzene, hexafluoro- (8CI9CI)

GB (exp) : 171.2 kcal/mol	Temperature : 373 K
PA (exp) : 178.5+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6HF5	CAS REGN : 363-72-4

```
      C
     . .
    .   .
F**C     C**F
   .     .
   .     .
F**C     C**F
    ..   .
     . .
      C
      *
      *
      F
```

Benzene, pentafluoro- (8CI9CI)

GB (exp) : 172.7+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.3+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H2F4	CAS REGN : 327-54-8

```
          F
          *
          *
       C..C
     .     .
   .         .
F**C         C**F
   .         .
     .     .
       C..C
       *
       *
       F
```

Benzene, 1,2,4,5-tetrafluoro- (8CI9CI)

GB (exp) : 173.1+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.3+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H2F4	CAS REGN : 551-62-2

```
      C
     . .
    .   .
F**C     C
   .     .
   .     .
F**C     C**F
    .   .
     . .
      C
      *
      *
      F
```

Benzene, 1,2,3,4-tetrafluoro- (8CI9CI)

GB (exp) : 173.4+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.4+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H2F4	CAS REGN : 2367-82-0

```
       C
      . .
     .   .
F**C     C**F
   .     .
   .     .
F**C     C
     .   .
      . .
       C
       *
       *
       F
```

Benzene, 1,2,3,5-tetrafluoro- (8CI9CI)

GB (exp) : 173.4+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.5+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H3F3	CAS REGN : 367-23-7

```
      C..C
     .    .
    .      .
F**C        C**F
    .      .
     .    .
      C..C
      *
      *
      F
```

Benzene, 1,2,4-trifluoro- (8CI9CI)

GB (exp) : 173.7+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.35+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H3F3	CAS REGN : 372-38-3

```
      F
      *
      *
      C
     . .
    .   .
   C     C
   .     .
   .     .
F**C     C**F
    .   .
     . .
      C
```

Benzene, 1,3,5-trifluoro- (8CI9CI)

GB (exp) : 174.1+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.15+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

Continued on next page

GB (exp) : 165.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 179.8+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C6H4F2	CAS REGN : 367-11-3

```
      C..C
     .    .
    .      .
F**C        C
    .      .
     .    .
      C..C
      *
      *
      F
```

Benzene, 1,2-difluoro- (9CI)
Benzene, o-difluoro- (8CI)

GB (exp) : 174.36+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.35+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H4F2	CAS REGN : 372-18-9

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
F**C     C**F
    .   .
     . .
      C
```

Benzene, 1,3-difluoro- (9CI)
Benzene, m-difluoro- (8CI)

GB (exp) : 174.42+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 171.67+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

Continued on next page

GB (exp) : 165.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 181.6+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C6H4F2	CAS REGN : 540-36-3

```
      C
     . .
    .   .
   C     C**F
   .     .
   .     .
F**C     C
    .   .
     . .
      C
```

Benzene, 1,4-difluoro- (9CI)
Benzene, p-difluoro- (8CI)

GB (exp) : 173.9+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 180.6+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

C6H4F3N	CAS REGN : 368-48-9

```
          C
         . .
        .   .
   F  N     C
   *  .     .
   *  .     .
F**C**C     C
   *   .   .
   *    . .
   F     C
```

Pyridine, 2-(trifluoromethyl)- (8CI9CI)

GB (exp) : 201.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.0+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H4F3N	CAS REGN : 3796-23-4

```
          N
         . .
        .   .
   F  C     C
   *  .     .
   *  .     .
F**C**C     C
   *   .   .
   *    . .
   F     C
```

Pyridine, 3-(trifluoromethyl)- (8CI)

GB (exp) : 202.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.0+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H4F3N	CAS REGN : 3796-24-5

```
          C
         . .
        .   .
   F  C     N
   *  .     .
   *  .     .
F**C**C     C
   *   .   .
   *    . .
   F     C
```

Pyridine, 4-(trifluoromethyl)- (8CI9CI)

GB (exp) : 202.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 207.1+/-2 kcal/mol	Temperature : 298 K

Taagepera, M., Henderson, W. G., Brownlee, R. T. C., Beauchamp, J. L., Holtz, D., and Taft, R. W., Gas-Phase Basicities and Pyridine Substituent Effects, J. Am. Chem. Soc. 94, 1369 (1972).

Method used : ICR
Equilibrium; scale based on C5H5N(Pyridine)

C6H4N2	CAS REGN : 100-48-1

```
          C
         . .
        .   .
       C     N
       .     .
       .     .
N##C**C     C
        .   .
         . .
          C
```

4-Pyridinecarbonitrile (9CI)
Isonicotinonitrile (8CI)

GB (exp) : 199.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 207.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H4N2	CAS REGN : 100-54-9

```
          N
         . .
       .     .
      C       C
      .       .
      .       .
N##C**C       C
       .     .
         . .
          C
```

3-Pyridinecarbonitrile (9CI)
Nicotinonitrile (8CI)

GB (exp) : 199.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H4N2	CAS REGN : 100-70-9

```
          C
         . .
        .   .
      N     C
      .     .
      .     .
N##C**C     C
        .   .
         . .
          C
```

2-Pyridinecarbonitrile (9CI)
Picolinonitrile (8CI)

GB (exp) : 197.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H5Cl	CAS REGN : 108-90-7

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
CL*C     C
    :   .
     . .
      C
```

Benzene, chloro- (8CI9CI)

GB (exp) : 174.24+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 181.9+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

Continued on next page

GB (exp) : 166.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.3+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes,
J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy
Equilbrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol

GB (exp) : 166.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.5+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C6H5F	CAS REGN : 462-06-6

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
F**C     C
    .   .
     . .
      C
```

Benzene, fluoro- (8CI9CI)

GB (exp) : 174.5+/-2 kcal/mol	Temperature : 373 K
PA (exp) : 182.2+/-2 kcal/mol	Temperature : 373 K

Hartman, K. G., and Lias, S. G.
Proton Transfer Equilibria in Halobenzene Systems:
Entropy Changes and Relative Proton Affinities,
Intern. J. Mass Spectrom. Ion Phys. 28, 213 (1978).

Method used : ICR
Calculated entropy
Equilibrium; scale based on C6H6

Continued on next page

GB (exp) : 167+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.5+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes,
J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy
Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol

GB (exp) : 166.9+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 182.6+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C6H5NO2	CAS REGN : 98-95-3

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
O++N**C     C
   +   .   .
   +     . .
   O     C
```

Benzene, nitro- (8CI9CI)

GB (exp) : 176.7+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 192.2+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes,
J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2

C6H6	CAS REGN : 71-43-2

```
   C..C
  .    .
 .      .
C        C
 .      .
  .    .
   C..C
```

Benzene (8CI9CI)

GB (exp) : 172+/-2 kcal/mol	Temperature : 340 K
PA (exp) : 180.1+/-2 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Proton Affinities of Benzene, Toluene, and the Xylenes,
J. Am. Chem. Soc. 94, 6630 (1972).

Method used : MS
Equilibrium relative to HCOOH
Entropy change assumed zero

GB (exp) : 174.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 181.4+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,
McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of
Compounds between Water and Ammonia from Pulsed Ion
Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 167.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 181.2+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

C6H6ClN	CAS REGN : 106-47-8

```
      C
     . .
    .   .
   C     C**N
   .     .
   .     .
CL*C     C
    .   .
     . .
      C
```

Benzenamine, 4-chloro- (9CI)
Aniline, p-chloro- (8CI)

GB (exp) : 198.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H6ClN	CAS REGN : 108-42-9

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
CL*C     C**N
    .   .
     . .
      C
```

Benzenamine, 3-chloro- (9CI)
Aniline, m-chloro- (8CI)

GB (exp) : 197.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H6FN	CAS REGN : 371-40-4

```
      C
     . .
    .   .
   C     C**N
   .     .
   .     .
F**C     C
    .   .
     . .
      C
```

Benzenamine, 4-fluoro- (9CI)
Aniline, p-fluoro- (8CI)

GB (exp) : 198.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H6FN	CAS REGN : 372-19-0

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
F**C     C**N
    .   .
     . .
      C
```

Benzenamine, 3-fluoro- (9CI)
Aniline, m-fluoro- (8CI)

GB (exp) : 197.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H6N4	CAS REGN : 2004-03-7

```
       C
      . .
     .   .
    N     N
    .     .
    .     .
C**C      C
     .   . %
      . .   %
       C     N
       *     %
       *     %
       N%%%%%C
```

1H-Purine, 6-methyl- (9CI)
Purine, 6-methyl- (8CI)

PA (exp) : 220+/-2 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)2NH and (CH3)3N

C6H6O	CAS REGN : 108-95-2

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
O**C     C
    .   .
     . .
      C
```

Phenol (8CI9CI)

PA (exp) : ~180 kcal/mol	Temperature :

DeFrees, D. J. McIver, R. T., and Hehre, W. J.
The Proton Affinities of Phenol,
J. Am. Chem. Soc. 99, 3853 (1977).

Method used : ICR
Bracketing relative to various molecules. Oxygen protonation

GB (exp) : 179.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes,
J. Am. Chem. Soc. 98, 7452 (1976).

Method used : ICR
Calculated entropy
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2

C6H6O	CAS REGN : 6921-27-3
C##C**C**O**C**C##C	
1-Propyne, 3,3'-oxybis- (9CI) 2-Propynyl ether (8CI)	
GB (exp) : 181.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.5+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H7N	CAS REGN : 62-53-3

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
N**C     C
    .   .
     . .
      C
```

Benzenamine (9CI)
Aniline (8CI)

GB (exp) : 200.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 193.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 208.9+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2

Continued on next page

GB (exp) : >193.7 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to NH3

GB (exp) : 194.0+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 211.2+/-2 kcal/mol	Temperature : 600 K

Briggs, J. P., Yamdagni, R., and Kebarle, P.,
Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton-Exchange Equilibria,
J. Am. Chem. Soc. 94, 5128 (1972).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

Continued on next page

GB (exp) : 199.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 203.9+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C6H7N	CAS REGN : 108-89-4

```
      C
     . .
    .   .
   C     N
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Pyridine, 4-methyl- (9CI)
4-Picoline (8CI)

GB (exp) : 214.30+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 222.10+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H7N	CAS REGN : 108-99-6

```
      N
     . .
    .   .
   C     C
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Pyridine, 3-methyl- (9CI)
3-Picoline (8CI)

GB (exp) : 213+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H7N	CAS REGN : 109-06-8

```
      C
     . .
    .   .
   N     C
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Pyridine, 2-methyl- (9CI)
2-Picoline (8CI)

GB (exp) : 213.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H7N	CAS REGN : 6921-28-4
C##C**C**N**C**C##C	
2-Propyn-1-amine, N-2-propynyl- (9CI) Di-2-propynylamine (8CI)	
GB (exp) : 205.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 213.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H7NO	CAS REGN : 620-08-6

```
          C
        . .
       .   .
      C     N
      .     .
      .     .
C**O**C     C
       .   .
        . .
          C
```

Pyridine, 4-methoxy- (8CI9CI)

GB (exp) : 217.00+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.80+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H7NO	CAS REGN : 694-85-9

```
      C++C
     *    *
    *      *
C**N         C
    *      +
     *    +
      C**C
      +
      +
      O
```

2(1H)-Pyridinone, 1-methyl- (9CI)
2(1H)-Pyridone, 1-methyl- (8CI)

PA (exp) : 217.2+/-2 kcal/mol	Temperature :

Cook, M. J., Katritzky, A. R., Taagepera, M., Singh, T. D., and Taft, R. W.
Application of Ion Cyclotron Resonance Spectroscopic Gas-Phase Basicities to the Study of Tautomeric Equilibria,
J. Am. Chem. Soc. 98, 6048 (1976).

Method used : ICR
Equilibrium relative to pyridine. Use value of PA (pyridine) = 210.1
Entropy change assumed zero

C6H7NO	CAS REGN : 1628-89-3

```
          C
        . .
       .   .
      N     C
      .     .
      .     .
C**O**C     C
       .   .
        . .
          C
```

Pyridine, 2-methoxy- (8CI9CI)

GB (exp) : 211.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 219.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

PA (exp) : 219.8+/-2 kcal/mol	Temperature :

Cook, M. J., Katritzky, A. R., Taagepera, M., Singh, T. D., and Taft, R. W.
Application of Ion Cyclotron Resonance Spectroscopic Gas-Phase Basicities to the Study of Tautomeric Equilibria,
J. Am. Chem. Soc. 98, 6048 (1976).

Method used : ICR
Equilibrium relative to t-Butylamine. Use value of PA (t-C4H9NH2) = 218.8
Entropy change assumed zero

C6H7NO	CAS REGN : 7295-76-3

```
          N
         . .
        .   .
      C     C
      .     .
      .     .
C**O**C     C
        .   .
         . .
          C
```

Pyridine, 3-methoxy- (8CI9CI)

GB (exp) : 213.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H7N5O	CAS REGN : 23662-75-1

```
C
 *
  *
   C%%N
   %   %
   %    %
   %     C..N
   %    .    .
   %   .      .
   N**C        C%%N
        .      .
         .    .
          C..N
          %
          %
          O
```

6H-Purin-6-one, 2-amino-1,7-dihydro-8-methyl- (9CI)
Guanine, 8-methyl- (8CI)

PA (exp) : >222 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)3N

C6H8N2	CAS REGN : 95-54-5

```
      C..C
     .    .
    .      .
N**C        C
    .      .
     .    .
      C..C
       *
       *
       N
```

1,2-Benzenediamine (9CI)
o-Phenylenediamine (8CI)

GB (exp) : >193.7 kcal/mol	Temperature : 424-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to NH3

C6H8N2	CAS REGN : 106-50-3

```
      C
     . .
    .   .
   C     C**N
   .     .
   .     .
N**C     C
    .   .
     . .
      C
```

1,4-Benzenediamine (9CI)
p-Phenylenediamine (8CI)

GB (exp) : >193.7 kcal/mol	Temperature : 424-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to NH3

C6H8N2	CAS REGN : 108-45-2

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
N**C     C**N
    .   .
     . .
      C
```

1,3-Benzenediamine (9CI)
m-Phenylenediamine (8CI)

GB (exp) : >202.9 kcal/mol	Temperature : 424-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to CH3NH2

C6H9F3O2	CAS REGN : 367-64-6

```
   F
   *
   *
F**C**C**O**C**C**C**C
   *  +
   *  +
   F  O
```

Acetic acid, trifluoro-, butyl ester (8CI9CI)

GB (exp) : 176.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 184.4+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H10	CAS REGN : 693-89-0

```
   C*****C
   +     *
   +     *
C**C     C
    *   *
     * *
      C
```

Cyclopentene, 1-methyl- (8CI9CI)

GB (exp) : 186.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 195+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H10	CAS REGN : 1528-30-9

```
   C*****C
   *     *
   *     *
C++C     C
    *   *
     * *
      C
```

Cyclopentane, methylene- (8CI9CI)

GB (exp) : 190.7+/-2 kcal/mol	Temperature : 298 K

Pollack, S. K., Wolf, J. F., Levi, B. A., Taft, R. W., and Hehre W. J.
Kinetic Detection of Common Intermediates in Gas Phase Ion-Molecule Reactions,
J. Am. Chem. Soc. 99, 1350 (1977).

Method used : ICR
Equilibrium; scale based on NH3

C6H10	CAS REGN : 4663-22-3

```
          C
         * *
        *   *
       C*****C
      *
     *
C**C
   +
   +
   C
```

Cyclopropane, (1-methylethenyl)- (9CI)
Propene, 2-cyclopropyl- (8CI)

GB (exp) : 198.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 207.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H10F3NO	CAS REGN : 400-59-9

```
   F
   *
   *
F**C**C%%N**C**C**C**C
   *  %
   *  %
   F  O
```

Acetamide, N-butyl-2,2,2-trifluoro- (8CI9CI)

GB (exp) : 193.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 201.7+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H10O	CAS REGN : 108-94-1

```
      C
     * *
    *   *
   C     C
   *     *
   *     *
O++C     C
    *   *
     * *
      C
```

Cyclohexanone (8CI9CI)

PA (exp) : 204 kcal/mol	Temperature :

Jelus, B. L., Murray, R. K., Jr., Munson, B.,
Studies in Chemical Ionization Mass Spectrometry.
Secondary Alcohols with Isobutane,
J. Am. Chem. Soc. 97, 2362 (1975).

Method used : MS
The (M-H)+ ion for cyclo-hexanol is assumed to be the same as O-protonated cyclohexanone.

C6H10O	CAS REGN : 557-40-4
C++C**C**O**C**C++C	
1-Propene, 3,3'-oxybis- (9CI) Allyl ether (8CI)	
GB (exp) : 190+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.4+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H11N	CAS REGN : 124-02-7
C++C**C**N**C**C++C	
2-Propen-1-amine, N-2-propenyl- (9CI) Diallylamine (8CI)	
GB (exp) : 213.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.8+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H11NO	CAS REGN : 931-20-4

```
      C**C
     *    *
    *      *
C**N         C
    *      *
     *    *
      C**C
      +
      +
      O
```

2-Piperidinone, 1-methyl- (9CI)
2-Piperidone, 1-methyl- (8CI)

PA (exp) : 216.8+/-2 kcal/mol	Temperature :

Cook, M. J., Katritzky, A. R., Taagepera, M., and Singh, T. D., and Taft, R. W.
Application of Ion Cyclotron Resonance Spectroscopic Gas-Phase Basicities to the Study of Tautomeric Equilibria,
J. Am. Chem. Soc. 98, 6048 (1976).

Method used : ICR
Equilibrium relative to i-C3H7NH2. Use value of PA (i-C3H7NH2) = 216.5
Entropy change assumed zero

C6H11NO	CAS REGN : 53687-79-9

```
          N
         + *
        +   *
       C     C
       *     *
       *     *
C**O***C     C
        *   *
         * *
          C
```

Piperidine, 2-methoxy-

PA (exp) : 226.3+/-2 kcal/mol	Temperature :

Cook, M. J., Katritzky, A. R., Taagepera, M., and Singh, T. D., and Taft, R. W.
Application of Ion Cyclotron Resonance Spectroscopic Gas-Phase Basicities to the Study of Tautomeric Equilibria,
J. Am. Chem. Soc. 98, 6048 (1976).

Method used : ICR
Equilibrium relative to (i-C3H7)2NH. Use value of PA(i-C3H7)2NH = 266.6
Entropy change assumed zero

C6H12	CAS REGN : Not available

```
      C
      *
      *
      C
      *
      *
C**C**C++C
```

1-Butene, 2-ethyl-

PA (exp) : 197.7+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Equilibrium of hydride transfer reaction between
(t-C4H9+) + Et2CHMe and between (t-C5H11+) + Et2CHMe.
This delta H of the reaction was determined from van't
Hoff plot. PA (M) derived from the obtained delta Hf(MH+);
scale based on delta Hf(t-C4H9+) = 169

C6H12	CAS REGN : 616-12-6

```
C**C++C**C**C
      *
      *
      C
```

2-Pentene, 3-methyl-, (E)- (8CI9CI)

PA (exp) : 196.1+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Equilibrium of hydride transfer reaction between
(t-C4H9+) + Et2CHMe and between (t-C5H11+) + Et2CHMe.
This delta H of the reaction was determined from van't
Hoff plot. PA (M) derived from the obtained delta Hf(MH+);
scale based on delta Hf(t-C4H9+) = 169

C6H12	CAS REGN : 625-27-4

```
C**C**C++C**C
          *
          *
          C
```

2-Pentene, 2-methyl- (8CI9CI)

PA (exp) : 196.4+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Equilibrium of hydride transfer Reaction between (t-C4H9+) + Me2CHC3H7 and between (t-C5H11+) + Me2CHC3H7. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169

C6H12	CAS REGN : 763-29-1

```
C**C**C**C**C
         +
         +
         C
```

i-Pentene, 2-methyl- (8CI9CI)

PA (exp) : 198.2+/-2 kcal/mol	Temperature : 363-553 K

Goren, A., and Munson, B.
Thermochemistry of Alkyl Ions,
J. Phys. Chem. 80, 2848 (1976).

Method used : MS
Equilibrium of hydride transfer reaction between (t-C4H9+) + Me2CHC3H7 and between (t-C5H11+) + Me2 CHC3H7. This delta H of the reaction was determined from van't Hoff plot. PA (M) derived from the obtained delta Hf(MH+); scale based on delta Hf(t-C4H9+) = 169

C6H12N2	CAS REGN : 280-57-9

```
   C**N
  *   **
 *   C  *
C    *   C
 *  C   *
  * *  *
   N**C
```

1,4-Diazabicyclo[2.2.2]octane (8CI9CI)

GB (exp) : 217.20+/-2 kcal/mol	Temperature :

Taft, R. W.,
Proton-Transfer Reactions,
Ed. E. F. Caldin and V. Gold,
(John Wiley and Sons, New York, 1975) Ch. 2.

Method used : ICR
Equilibrium; scale based on NH3

GB (exp) : 217.90+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.90+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

Continued on next page

PA (exp) : 225.50+/-2 kcal/mol	Temperature :

Staley, R., and Beauchamp, J. L.,
Relationship of Nitrogen Lone Pair Interactions
to Thermodynamic Parameters Associated with Amine
Basicities,
J. Am. Chem. Soc. 96, 1604 (1974).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H12O	CAS REGN : 75-97-8

```
   C
   *
   *
C**C**C**C
   *  +
   *  +
   C  O
```

2-Butanone, 3,3-dimethyl- (8CI9CI)

GB (exp) : 191.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H12O2	CAS REGN : 598-98-1

```
         C
         *
         *
C**O**C**C**C
      +  *
      +  *
      O  C
```

Propanoic acid, 2,2-dimethyl-, methyl ester (9CI)
Pivalic acid, methyl ester (8CI)

GB (exp) : 192.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H13N	CAS REGN : 108-91-8

```
      C
     * *
    *   *
   C     C
   *     *
   *     *
N**C     C
    *   *
     * *
      C
```

Cyclohexanamine (9CI)
Cyclohexylamine (8CI)

GB (exp) : 210.10+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 218.5+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 210.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 218.5+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

Continued on next page

GB (exp) : 204.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 222+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding
in Proton-Bound Amine Dimers and Proton-Induced
Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C6H13N	CAS REGN : 626-67-5

```
      C
     * *
    *   *
   C     C
   *     *
   *     *
C**N     C
    *   *
     * *
      C
```

Piperidine, 1-methyl- (8CI9CI)

GB (exp) : 218.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 218.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 226.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C6H14O	CAS REGN : 108-20-3

```
C**C**O**C**C
   *     *
   *     *
   C     C
```

Propane, 2,2'-oxybis- (9CI)
Isopropyl ether (8CI)

GB (exp) : 195.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera,
McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H14O	CAS REGN : 111-43-3
C**C**C**O**C**C**C	
Propane, 1,1'-oxybis- (9CI) Propyl ether (8CI)	
GB (exp) : 191.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.3+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H14O	CAS REGN : 637-92-3

```
        C
        *
        *
C**C**O**C**C
        *
        *
        C
```

Propane, 2-ethoxy-2-methyl- (9CI)
Ether, tert-butyl ethyl (8CI)

GB (exp) : 195.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H14S	CAS REGN : 111-47-7
C**C**C**S**C**C**C	
Propane, 1,1'-thiobis- (9CI) Propyl sulfide (8CI)	
GB (exp) : 196.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

C6H14S	CAS REGN : 625-80-9

```
C**C**S**C**C
   *     *
   *     *
   C     C
```

Propane, 2,2'-thiobis- (9CI)
Isopropyl sulfide (8CI)

GB (exp) : 199.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 206.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H15N	CAS REGN : 108-18-9

```
C**C**N**C**C
   *      *
   *      *
   C      C
```

2-Propanamine, N-(1-methylethyl)- (9CI)
Diisopropylamine (8CI)

GB (exp) : 218.40+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.60+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 217.90+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 226.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C6H15N	CAS REGN : 111-26-2
N**C**C**C**C**C**C	
1-Hexanamine (9CI) Hexylamine (8CI)	
GB (exp) : 208.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.5+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C6H15N	CAS REGN : 121-44-8

```
C**C**N**C**C
      *
      *
      C
      *
      *
      C
```

Ethanamine, N,N-diethyl- (9CI)
Triethylamine (8CI)

GB (exp) : 221.20+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 229.00+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 220.60+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 228.40+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C6H15N	CAS REGN : 142-84-7
C**C**C**N**C**C**C	
1-Propanamine, N-propyl- (9CI) Dipropylamine (8CI)	
GB (exp) : 216.50+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 224.70+/-2 kcal/mol	Temperature : 300 K
Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	
GB (exp) : 216.10+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 224.30+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C6H15N	CAS REGN : 918-02-5

```
   C
   *
   *
C**C**N**C
   *  *
   *  *
   C  C
```

2-Propanamine, N,N,2-trimethyl- (9CI)
Ethylamine, N,N,1,1-tetramethyl- (8CI)

GB (exp) : 220.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C6H16N2	CAS REGN : 110-18-9

```
C**N**C**C**N**C
   *        *
   *        *
   C        C
```

1,2-Ethanediamine, N,N,N',N'-tetramethyl- (9CI)
Ethylenediamine, N,N,N',N'-tetramethyl- (8CI)

GB (exp) : 224.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 232.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 224+/-2 kcal/mol	Temperature : 298 K

Taft, R. W.,
Proton-Transfer Reactions,
Ed. E. F. Caldin and V. Gold,
(John Wiley and Sons, New York, 1975) Ch. 2.

Method used : ICR
Equilibrium; scale based on NH3

C6H16N2	CAS REGN : 124-09-4
N**C**C**C**C**C**C**N	
1,6-Hexanediamine (8CI9CI)	
GB (exp) : 220.00+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.40+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Evaluation of Intramolecular Strong Hydrogen Bonding in the Gas Phase, J. Am. Chem. Soc. 95, 2669 (1973).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	
GB (exp) : 221.20+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 235.00+/-2 kcal/mol	Temperature : 298 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on (CH3)3N Van't Hoff plot	

C6H17NSi	CAS REGN : 18182-40-6

```
          C
          *
          *
C**N**C**SI*C
   *      *
   *      *
   C      C
```

Methanamine, N,N-dimethyl-1-(trimethylsilyl)- (9CI)
Trimethylamine, (trimethylsilyl)- (8CI)

GB (exp) : 219.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 227.7+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H5ClO	CAS REGN : 104-88-1

```
          C
         . .
       .     .
      C       C**CL
      .       .
      .       .
O++C**C       C
       .     .
         . .
          C
```

Benzaldehyde, 4-chloro- (9CI)
Benzaldehyde, p-chloro- (8CI)

GB (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H5D3	CAS REGN : 1124-18-1

```
   C     D
  . .    *
 .   .   *
C     C**C**D
.     .  *
.     .  *
C     C  D
 .   .
  . .
   C
```

Benzene, methyl-d3-

GB (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.7+/-2 kcal/mol	Temperature : 300 K

Ausloos, P., and Lias, S. G.
Equilibrium Isotope Effects on the Proton Transfer Reactions of Methylbenzenes,
J. Am. Chem. Soc. 99, 4198 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H5FO	CAS REGN : 456-48-4

```
          C
        . .
       .   .
      C     C
      .     .
      .     .
O++C**C     C**F
       .   .
        . .
          C
```

Benzaldehyde, 3-fluoro- (9CI)
Benzaldehyde, m-fluoro- (8CI)

GB (exp) : 186.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 194.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H5FO	CAS REGN : 459-57-4

```
          C
         . .
       .     .
      C       C**F
      .       .
      .       .
O++C**C       C
       .     .
         . .
          C
```

Benzaldehyde, 4-fluoro- (9CI)
Benzaldehyde, p-fluoro- (8CI)

GB (exp) : 188.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.7+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H5N	CAS REGN : 100-47-0

```
          C
         . .
       .     .
      C       C
      .       .
      .       .
N##C**C       C
       .     .
         . .
          C
```

Benzonitrile (8CI9CI)

GB (exp) : 179.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 194.7+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2

C7H6O	CAS REGN : 100-52-7

```
          C
         . .
       .     .
      C       C
      .       .
      .       .
O++C**C       C
       .     .
         . .
          C
```

Benzaldehyde (8CI9CI)

GB (exp) : 190.4 kcal/mol	Temperature : 300 K
PA (exp) : 198.2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 183.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 198.7+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2

C7H7NO	CAS REGN : 350-03-8

```
          N
         . .
       C     C
       .     .
       .     .
C**C**C      C
   +   .   .
   +     . .
   O      C
```

Ethanone, 1-(3-pyridinyl)- (9CI)
Ketone, methyl 3-pyridyl (8CI)

GB (exp) : 206.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H7NO	CAS REGN : 1122-54-9

```
          C
         . .
        .   .
       C     N
       .     .
       .     .
C**C**C      C
   +    .   .
   +     . .
   O      C
```

Ethanone, 1-(4-pyridinyl)- (9CI)
Ketone, methyl 4-pyridyl (8CI)

GB (exp) : 206.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H8	CAS REGN : 108-88-3

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Benzene, methyl- (9CI)
Toluene (8CI)

GB (exp) : 179.6+/-2 kcal/mol	Temperature : 340 K
PA (exp) : 187.5+/-2 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Proton Affinities of Benzene, Toluene, and the Xylenes,
J. Am. Chem. Soc. 94, 6630 (1972).

Method used : MS
Equilibrium relative to CH3SH
Entropy change assumed zero

PA (exp) : 187.4+/-2 kcal/mol	Temperature : 300 K

Devlin, J. L., III., Wolf, J. F., Taft, R. W.,
Hehre, W. J.,
The Proton Affinities of Toluene,
J. Am. Chem. Soc. 98, 1990 (1976).

Method used : ICR
Equilibrium relative to C6H6(Benzene)
Protonation position 2

Continued on next page

PA (exp) : 183.8+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III., Wolf, J. F., Taft, R. W., Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Equilibrium relative to C6H6(Benzene) Protonation position 3	
PA (exp) : 182.6+/-2 kcal/mol	Temperature : 300 K
Devlin, J. L., III., Wolf, J. F., Taft, R. W., Hehre, W. J., The Proton Affinities of Toluene, J. Am. Chem. Soc. 98, 1990 (1976).	
Method used : ICR Equilibrium relative to C6H6(Benzene) Protonation position 1	
GB (exp) : 174.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 189.6+/-2 kcal/mol	Temperature : 600 K
Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).	
Method used : MS Calculated entropy Equilibrium relative to C6H6. Using GB and PA values respectively 167.8+/-2 and 181.2+/-2 kcal/mol	

Continued on next page

GB (exp) : 180.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.6+/-2 kcal/mol	Temperature : 300 K

Devlin, J. L., III., Wolf, J. F., Taft, R. W.,
Hehre, W. J.,
The Proton Affinities of Toluene,
J. Am. Chem. Soc. 98, 1990 (1976).

Method used : ICR
Protonation position 4
Calculated entropy
Equilibrium relative to C6H6(Benzene)

GB (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 188.7+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M.,
McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of
Compounds between Water and Ammonia from Pulsed Ion
Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

Continued on next page

GB (exp) : 180.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.9+/-2 kcal/mol	Temperature : 300 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on C6H6(Benzene)

C7H8O	CAS REGN : 100-66-3

```
          C
         . .
        .   .
       C     C
       .     .
       .     .
C**O**C     C
        .   .
         . .
          C
```

Benzene, methoxy- (9CI)
Anisole (8CI)

GB (exp) : 183.5+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 199+/-2 kcal/mol	Temperature : 600 K

Lau, Y. K., and Kebarle, P.
Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).

Method used : MS
Calculated entropy .
Equilibrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2

C7H9N	CAS REGN : 100-46-9

```
          C
         . .
       .     .
      C       C
      .       .
      .       .
N**C**C       C
       .     .
         . .
          C
```

Benzenemethanamine (9CI)
Benzylamine (8CI)

GB (exp) : 206.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.5+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9N	CAS REGN : 100-61-8

```
          C
         . .
        .   .
       C     C
       .     .
       .     .
C**N**C     C
        .   .
         . .
          C
```

Benzenamine, N-methyl- (9CI)
Aniline, N-methyl- (8CI)

GB (exp) : 200.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 217.4+/-2 kcal/mol	Temperature : 600 K

Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton-Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C7H9N	CAS REGN : 106-49-0

```
      C
     . .
    .   .
   C     C**N
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Benzenamine, 4-methyl- (9CI)
p-Toluidine (8CI)

GB (exp) : 203.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9N	CAS REGN : 108-44-1

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
C**C     C**N
    ..   .
     . .
      C
```

Benzenamine, 3-methyl- (9CI)
m-Toluidine (8CI)

GB (exp) : 203.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 211.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 211.6+/-2 kcal/mol	Temperature : 298 K

Pollack, S. K., Devlin, J. L., III, Summerhays, K. D., Taft, R. W., and Hehre, W J.
The Site of Protonation in Aniline,
J. Am. Chem. Soc. 99, 4583 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3. Ring protonation

Continued on next page

PA (exp) : 211.6+/-2 kcal/mol	Temperature : 300 K

Summerhays, K. D., Pollack, S. K., Taft, R. W., and Hehre, W. J.
Gas-Phase Basicities of Substituted Anilines. Inferences about the Role of Solvent in Dictating Site of Protonation,
J. Am. Chem. Soc. 99, 4585 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale base on NH3. Ring protonation

C7H9N	CAS REGN : 108-47-4

```
      C
     . .
    .   .
   C     N
   .     .
   .     .
C**C     C**C
    .   .
     . .
      C
```

Pyridine, 2,4-dimethyl- (9CI)
2,4-Lutidine (8CI)

PA (exp) : 225.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr.
A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines,
J. Am. Chem. Soc. 98, 854 (1976).

Method used : ICR
Calculated Entropy
Equilibrium; scale based on NH3

C7H9N	CAS REGN : 108-48-5

```
       C
      . .
    .     .
   C       C
   .       .
   .       .
C**C       C**C
    .     .
      . .
       N
```

Pyridine, 2,6-dimethyl- (9CI)
2,6-Lutidine (8CI)

PA (exp) : 226.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr.
A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines,
J. Am. Chem. Soc. 98, 854 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9N	CAS REGN : 589-93-5

```
      N
     . .
    .   .
   C     C**C
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Pyridine, 2,5-dimethyl- (9CI)
2,5-Lutidine (8CI)

PA (exp) : 224.5+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr.
A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines,
J. Am. Chem. Soc. 98, 854 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9N	CAS REGN : 591-22-0

```
      N
     . .
    .   .
   C     C
   .     .
   .     .
C**C     C**C
    .   .
     . .
      C
```

Pyridine, 3,5-dimethyl- (9CI)
3,5-Lutidine (8CI)

PA (exp) : 223.5 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., Bowers, M. T., Liotta, C. L., Alexander, C. J., and Hopkins, H. P., Jr.
A Quantitative Comparison of Gas- and Solution-Phase Basicities of Substituted Pyridines,
J. Am. Chem. Soc. 98, 854 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9NO	CAS REGN : 90-04-0

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
C**O**C     C
        .   .
         . .
          C
          *
          *
          N
```

Benzenamine, 2-methoxy- (9CI)
o-Anisidine (8CI)

GB (exp) : 200.2+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 217.4+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Entropy change assumed zero
Equilibrium; scale based on CH3NH2

C7H9NO	CAS REGN : 104-94-9

```
          C
         . .
        .   .
       C     C**N
       .     .
       .     .
C**O**C     C
        .   .
         . .
          C
```

Benzenamine, 4-methoxy- (9CI)
p-Anisidine (8CI)

GB (exp) : 203.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H9NO	CAS REGN : 536-90-3

```
          C
         . .
       .     .
      C       C
      .       .
      .       .
C**O**C       C**N
       .     .
         . .
          C
```

Benzenamine, 3-methoxy- (9CI)
m-Anisidine (8CI)

PA (exp) : 214.0+/-2 kcal/mol	Temperature : 300 K

Summerhays, K. D., Pollack, S. K., Taft, R. W., and Hehre, W. J.
Gas-Phase Basicities of Substituted Anilines. Inferences about the Role of Solvent in Dictating Site of Protonation,
J. Am. Chem. Soc. 99, 4585 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale base on NH3. Ring protonation

C7H10	CAS REGN : 498-66-8

```
C*****C
*     *
*     *
C*C+C*C
 *   *
  * *
   C
```

Bicyclo[2.2.1]hept-2-ene (9CI)
2-Norbornene (8CI)

PA (exp) : 198.8+/-2 kcal/mol	Temperature : 300 K

Staley, R. H., Wieting, R. D., and Beauchamp, J. L.
Carbenium Ion Stabilities in the Gas Phase and Solution. An Ion Cyclotron Resonance Study of Bromide Transfer Reactions Involving Alkali Ions, Alkyl Carbenium Ions, Acyl Cations, and Cyclic Halonium Ions,
J. Am. Chem. Soc. 99, 5964 (1977).

Method used : ICR
Calculated entropy
Equilibrium relative to Et2O; scale based on NH3

C7H10N2	CAS REGN : 1122-58-3

```
          C
         . .
        .   .
      C     N
      .     .
      .     .
C**N**C     C
   *   .   .
   *     . .
   C     C
```

4-Pyridinamine, N,N-dimethyl- (9CI)
Pyridine, 4-(dimethylamino)- (8CI)

GB (exp) : 224.90+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 232.70+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to (CH3)2NH

C7H12	CAS REGN : 591-49-1

```
      C
     * *
    *   *
   C     C
   +     *
   +     *
C**C     C
    *   *
     * *
      C
```

Cyclohexene, 1-methyl- (8CI9CI)

GB (exp) : 188.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 196.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H12	CAS REGN : 765-47-9

```
   C*****C
   *     *
   *     *
C**C     C
    +   *
     + *
      C
      *
      *
      C
```

Cyclopentene, 1,2-dimethyl- (8CI9CI)

GB (exp) : 188.4+/-2 kcal/mol	Temperature : 298 K

Pollack, S. K., Wolf, J. F., Levi, B. A., Taft, R. W., and Hehre, W. J.
Kinetic Detection of Common Intermediates in Gas Phase Ion-Molecule Reactions,
J. Am. Chem. Soc. 99, 1350 (1977).

Method used : ICR

C7H13N	CAS REGN : 100-76-5

```
   C**N
  *   **
 *   C  *
C    *   C
 *  C   *
  * *  *
   C**C
```

1-Azabicyclo[2.2.2]octane (9CI)
Quinuclidine (8CI)

GB (exp) : 220.80+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.60+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 220.80+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 228.60+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

Continued on next page

GB (exp) : 209.7 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines,
Anilines, and Pyridines. An Application of Some
Bronsted Acids as Reactants in Chemical Ionization
Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to (CH3)2NH

C7H17N	CAS REGN : 111-68-2

C**C**C**C**C**C**C**N

1-Heptanamine (9CI)
Heptylamine (8CI)

GB (exp) : 208.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 216.5+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Evaluation of Intramolecular Strong
Hydrogen Bonding in the Gas Phase,
J. Am. Chem. Soc. 95, 2669 (1973).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C7H17N	CAS REGN : 4458-31-5

```
C**C**N**C**C**C
      *
      *
      C
      *
      *
      C
```

1-Propanamine, N,N-diethyl- (9CI)
Propylamine, N,N-diethyl- (8CI)

GB (exp) : 221.3+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 229.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C7H17N	CAS REGN : 10076-31-0

```
          C
          *
          *
C**N**C**C**C
   *      *
   *      *
   C      C
```

1-Propanamine, N,N,2,2-tetramethyl- (9CI)
Propylamine, N,N,2,2-tetramethyl- (8CI)

GB (exp) : 218.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C7H18N2	CAS REGN : 110-95-2

```
C**N**C**C**C**N**C
   *          *
   *          *
   C          C
```

1,3-Propanediamine, N,N,N',N'-tetramethyl- (8CI9CI)

GB (exp) : 227.7+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Equilibrium; scale based on NH3

C8H4D6	CAS REGN : 25493-13-4

```
   D     C
   *    . .
   *   .   .
D**C**C     C  D
   *  .     .  *
   *  .     .  *
   D  C     C**C**D
       .   .    *
        . .     *
         C      D
```

Benzene, 1,4-(dimethyl-d3)-

GB (exp) : 182.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K

Ausloos, P., and Lias, S. G.
Equilibrium Isotope Effects on the Proton Transfer Reactions of Methylbenzenes,
J. Am. Chem. Soc. 99, 4198 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H5F3O	CAS REGN : 455-19-6

```
          C
         . .
        .   .
   F  C     C**C++O
   *  .     .
   *  .     .
F**C**C     C
   *   .   .
   *    . .
   F     C
```

Benzaldehyde, 4-(trifluoromethyl)- (9CI)
p-Tolualdehyde, .alpha.,.alpha.,.alpha.-trifluoro- (8CI)

GB (exp) : 181.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H5NO	CAS REGN : 105-07-7

```
          C
         . .
       .     .
      C       C**C++O
      .       .
      .       .
N##C**C       C
       .     .
         . .
          C
```

Benzonitrile, 4-formyl- (9CI)
Terephthalaldehydonitrile (8CI)

GB (exp) : 177.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 185.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8	CAS REGN : 100-42-5

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
C++C**C     C
        .   .
         . .
          C
```

Benzene, ethenyl- (9CI)
Styrene (8CI)

GB (exp) : 191.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 199.3+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8O	CAS REGN : 98-86-2

```
          C
         . .
       .     .
      C       C
      .       .
      .       .
C**C**C       C
   +  .     .
   +     . .
   O      C
```

Ethanone, 1-phenyl- (9CI)
Acetophenone (8CI)

GB (exp) : 195.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8O	CAS REGN : 104-87-0

```
          C
         . .
       .     .
      C       C**C
      .       .
      .       .
O++C**C       C
       .     .
         . .
          C
```

Benzaldehyde, 4-methyl- (9CI)
p-Tolualdehyde (8CI)

GB (exp) : 194+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 201.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8O2	CAS REGN : 93-58-3

```
            C
           . .
          .   .
         C     C
         .     .
         .     .
C**O**C**C     C
      +   .   .
      +    . .
      O     C
```

Benzoic acid, methyl ester (8CI9CI)

GB (exp) : 193.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 200.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H8O2	CAS REGN : 123-11-5

```
          C
         . .
       .     .
      C       C**O**C
      .       .
      .       .
O++C**C       C
       .     .
         . .
          C
```

Benzaldehyde, 4-methoxy- (9CI)
p-Anisaldehyde (8CI)

GB (exp) : 203.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H10	CAS REGN : 95-47-6

```
      C..C
     .    .
    .      .
C**C        C
    .      .
     .    .
      C..C
       *
       *
       C
```

Benzene, 1,2-dimethyl- (9CI)
o-Xylene (8CI)

GB (exp) : 183+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 190+/-3 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Proton Affinities of Benzene, Toluene, and the Xylenes,
J. Am. Chem. Soc. 94, 6630 (1972).

Method used : MS
Equilibrium relative to CH3SH and (CH3)2O
Entropy change assumed zero

Continued on next page

GB (exp) : 183.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 191.1+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia From Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H10	CAS REGN : 100-41-4

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
C**C**C     C
        .   .
         . .
          C
```

Benzene, ethyl- (8CI9CI)

GB (exp) : 181.8+/-2 kcal/mol	Temperature : 300 K

Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).

Method used : ICR
Equilibrium; scale based on C6H5CH3(Toluene)

Continued on next page

GB (exp) : 175.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 600 K
Lau, Y. K., and Kebarle, P. Substituent Effects on the Intrinsic Basicity of Benzene: Proton Affinities of Substituted Benzenes, J. Am. Chem. Soc. 98, 7452 (1976).	
Method used : MS Calculated entropy Equilbrium relative to C6H6. Using GB (C6H6) = 167.8+/-2 and PA (C6H6) = 181.2+/-2	
GB (exp) : 180.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.1+/-2 kcal/mol	Temperature : 300 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : MS Calculated entropy Equilibrium; scale based on C6H6(Benzene)	

Continued on next page

GB (exp) : 181.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.6+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H10	CAS REGN : 106-42-3

```
      C
     . .
    .   .
   C     C**C
   .     .
   .     .
C**C     C
    .   .
     . .
      C
```

Benzene, 1,4-dimethyl- (9CI)
p-Xylene (8CI)

GB (exp) : 182+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 189+/-3 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Proton Affinities of Benzene, Toluene, and the Xylenes,
J. Am. Chem. Soc. 94, 6630 (1972).

Method used : MS
Equilibrium; scale based on CH3SH and (CH3)2O
Entropy change assumed zero

GB (exp) : 182.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 189.8+/-2 kcal/mol	Temperature : 300 K

Devlin, J. L., III, Wolf, J. F., Taft, R. W., and
Hehre, W. J.,
The Proton Affinities of Toluene,
J. Am. Chem. Soc. 98, 1990 (1976).

Method used : ICR
Calculated entropy
Equilibrium relative to C6H6(Benzene)

C8H10	CAS REGN : 108-38-3

```
      C
     . .
    .   .
   C     C
   .     .
   .     .
C**C     C**C
    .   .
     . .
      C
```

Benzene, 1,3-dimethyl- (9CI)
m-Xylene (8CI)

GB (exp) : 182+/-3 kcal/mol	Temperature : 340 K
PA (exp) : 189.7+/-3 kcal/mol	Temperature : 340 K

Chong, S. L., and Franklin, J. L.,
Proton Affinities of Benzene, Toluene, and the Xylenes,
J. Am. Chem. Soc. 94, 6630 (1972).

Method used : MS
Equilibrium relative to CH3SH and (CH3)2O
Entropy change assumed zero

GB (exp) : 187.2+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 194.6+/-2 kcal/mol	Temperature : 298 K

Devlin, J. L., III, Wolf, J. F., Taft, R. W., and
Hehre, W. J.,
The Proton Affinities of Toluene,
J. Am. Chem. Soc. 98, 1990 (1976).

Method used : ICR
Calculated entropy
Equilibrium relative to C6H6(Benzene)

C8H11N	CAS REGN : 103-69-5

```
            C
           . .
          .   .
         C     C
         .     .
         .     .
C**C**N**C     C
          .   .
           . .
            C
```

Benzenamine, N-ethyl- (9CI)
Aniline, N-ethyl- (8CI)

GB (exp) : 203.6+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 220.8+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : ICR
Equilibrium; scale based on NH3
Entropy change assumed zero

C8H11N	CAS REGN : 121-69-7

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
C**N**C     C
   *  .   .
   *    . .
   C     C
```

Benzenamine, N,N-dimethyl- (9CI)
Aniline, N,N-dimethyl- (8CI)

GB (exp) : 212.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 220.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

PA (exp) : 220+/-2 kcal/mol	Temperature : 298 K

Pollack, S. K., Devlin, J. L., III, Summerhays, K. D., Taft, R. W., and Hehre, W. J.
The Site of Protonation in Aniline,
J. Am. Chem. Soc. 99, 4583 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3. Protonation on the nitrogen

Continued on next page

GB (exp) : 206.8+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 224+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines, J. Am. Chem. Soc. 95, 3504 (1973).	
Method used : MS Equilibrium; scale based on NH3 Entropy change assumed zero	
GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K
Dzidic, I., Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry, J. Am. Chem. Soc. 94, 8333 (1972).	
Method used : MS Bracketing relative to (CH3)2NH	

C8H18S	CAS REGN : 107-47-1

```
   C     C
   *     *
   *     *
C**C**S**C**C
   *     *
   *     *
   C     C
```

Propane, 2,2'-thiobis[2-methyl- (9CI)
tert-Butyl sulfide (8CI)

GB (exp) : 203.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 210.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H19N	CAS REGN : 110-96-3

```
C**C**C**N**C**C**C
   *          *
   *          *
   C          C
```

1-Propanamine, 2-methyl-N-(2-methylpropyl)- (9CI)
Diisobutylamine (8CI)

GB (exp) : 217.7+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.9+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C8H19N	CAS REGN : 111-92-2
C**C**C**C**N**C**C**C**C	
1-Butanamine, N-butyl- (9CI) Dibutylamine (8CI)	
GB (exp) : 217.20+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 225.40+/-2 kcal/mol	Temperature : 298 K
Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Proton Affinities, Ionization Potentials, and Hydrogen Affinities of Alkylamines, J. Am. Chem. Soc. 98, 311 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on CH3NH2	

C8H19N	CAS REGN : 626-23-3

```
C**C**C**N**C**C**C
      *     *
      *     *
      C     C
```

2-Butanamine, N-(1-methylpropyl)- (9CI)
Di-sec-butylamine (8CI)

GB (exp) : 219.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 228.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C8H19N	CAS REGN : 7087-68-5

```
C**C**N**C**C
   *  *  *
   *  *  *
   C  C  C
      *
      *
      C
```

2-Propanamine, N-ethyl-N-(1-methylethyl)- (9CI)
Triethylamine, 1,1'-dimethyl- (8CI)

GB (exp) : 223.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 231.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H19N	CAS REGN : 21981-37-3

```
   C     C
   *     *
   *     *
C**C**N**C**C
   *     *
   *     *
   C     C
```

2-Propanamine, N-(1,1-dimethylethyl)-2-methyl- (9CI)
Di-tert-butylamine (8CI)

GB (exp) : 221.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 229.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C8H20N2	CAS REGN : 111-51-3

```
C**N**C**C**C**C**N**C
   *            *
   *            *
   C            C
```

1,4-Butanediamine, N,N,N',N'-tetramethyl- (8CI9CI)

GB (exp) : 229.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Equilibrium; scale based on NH3

C9H9Cl	CAS REGN : 1712-70-5

```
          C
         . .
        .   .
      C     C**CL
      .     .
      .     .
C**C**C     C
   +   .   .
   +     . .
   C     C
```

Benzene, 1-chloro-4-(1-methylethenyl)- (9CI)
Styrene, p-chloro-.alpha.-methyl- (8CI)

GB (exp) : 195.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 203+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H9F	CAS REGN : 350-40-3

```
          C
         . .
        .   .
      C     C**F
      .     .
      .     .
C**C**C     C
   +   .   .
   +     . .
   C     C
```

Benzene, 1-fluoro-4-(1-methylethenyl)- (9CI)
Styrene, p-fluoro-.alpha.-methyl- (8CI)

GB (exp) : 196.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 204.7+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H9N	CAS REGN : 6921-29-5

```
C##C**C**N**C**C##C
         *
         *
         C
         *
         *
         C
         #
         #
         C
```

2-Propyn-1-amine, N,N-di-2-propynyl- (9CI)
Tri-2-propynylamine (8CI)

GB (exp) : 209.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 217.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H10	CAS REGN : 98-83-9

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
C**C**C     C
   +  .   .
   +     . .
   C     C
```

Benzene, (1-methylethenyl)- (9CI)
Styrene, .alpha.-methyl- (8CI)

GB (exp) : 197.0+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H12	CAS REGN : 98-82-8

```
          C
         . .
        .   .
      C     C
      .     .
      .     .
C**C**C     C
   *   .   .
   *     . .
   C     C
```

Benzene, (1-methylethyl)- (9CI)
Cumene (8CI)

GB (exp) : 183+/-2 kcal/mol	Temperature : 300 K

Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).

Method used : ICR
Equilibrium; scale based on C6H5CH3(Toluene)

Continued on next page

GB (exp) : 182.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.4+/-2 kcal/mol	Temperature : 300 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on C6H6(Benzene)

C9H12	CAS REGN : 103-65-1

```
            C
           . .
          .   .
         C     C
         .     .
         .     .
C**C**C**C     C
          .   .
           . .
            C
```

Benzene, propyl- (8CI9CI)

GB (exp) : 182.6+/-2 kcal/mol	Temperature : 300 K

Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).

Method used : ICR
Equilibrium; scale based on C6H5CH3(Toluene)

Continued on next page

GB (exp) : 181.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190+/-2 kcal/mol	Temperature : 300 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on C6H6(Benzene)

GB (exp) : 182.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.4+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H12	CAS REGN : 108-67-8

```
      C
      *
      *
      C
     . .
    .   .
   C     C
   .     .
   .     .
C**C     C**C
    .   .
     . .
      C
```

Benzene, 1,3,5-trimethyl- (9CI)
Mesitylene (8CI)

GB (exp) : 191.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 198.4+/-2 kcal/mol	Temperature : 300 K

Devlin, J. L., III, Wolf, J. F., Taft, R. W., and Hehre, W. J.,
The Proton Affinities of Toluene,
J. Am. Chem. Soc. 98, 1990 (1976).

Method used : ICR
Calculated entropy
Equilibrium relative to benzene

C9H12N2O6	CAS REGN : 58-96-8

```
                              O
                              *
                              *
                              C
                             *
                            *
      C++C             O**C
     *    *           *   *
    *      *         *    *
O%%C         N*****C      *
   %       *         *    *
    %    *           *   *
     N%%C             C**C
        %             *   *
        %             *    *
        O             O     O
```

Uridine (8CI9CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C9H13N	CAS REGN : 121-72-2

```
          C
         . .
        .   .
       C     C
       .     .
       .     .
C**N**C      C**C
   *   .   .
   *     . .
   C     C
```

Benzenamine, N,N,3-trimethyl- (9CI)
m-Toluidine, N,N-dimethyl- (8CI)

PA (exp) : 221+/-2 kcal/mol	Temperature : 298 K

Pollack, S. K., Devlin, J. L., III, Summerhays, K. D.
Taft, R. W., and Hehre, W. J.
The Site of Protonation in Aniline,
J. Am. Chem. Soc. 99, 4583 (1977).

Method used : ICR
Equilibrium; scale based on NH3. Protonation on the nitrogen

C9H13N	CAS REGN : 613-97-8

```
            C
           . .
          .   .
         C     C
         .     .
         .     .
C**C**N**C     C
      *   .   .
      *    . .
      C     C
```

Benzenamine, N-ethyl-N-methyl- (9CI)
Aniline, N-ethyl-N-methyl- (8CI)

GB (exp) : 209.40+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 226.60+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Entropy change assumed zero
Equilibrium; scale based on NH3

C9H13N3O5	CAS REGN : 65-46-3

```
                              O
                              *
                              *
                              C
                             *
                            *
       C++C             O**C
     *    *           *   *
    *      *         *    *
N%%C         N*****C      *
    %      *        *    *
     %    *          *   *
      N%%C            C**C
         %            *   *
         %            *    *
         O            O     O
```

Cytidine (9CI)

PA (exp) : >222 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)3N.

C9H14N2O6	CAS REGN : 5627-05-4

```
                              O
                              *
                              *
                              C
                             *
                            *
       C**C              O**C
      *    *            *   *
     *      *          *    *
O%%C         N*****C        *
     %      *          *    *
      %    *            *   *
       N%%C              C**C
          %              *   *
          %              *    *
          O              O     O
```

Uridine, 5,6-dihydro- (9CI)
Hydrouracil, 1-.beta.-D-ribofuranosyl- (8CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C9H15N	CAS REGN : 102-70-5

```
C++C**C**N**C**C++C
         *
         *
         C
         *
         *
         C
         +
         +
         C
```

2-Propen-1-amine, N,N-di-2-propenyl- (9CI)
Triallylamine (8CI)

GB (exp) : 219+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 226.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C9H21N	CAS REGN : 102-69-2

```
C**C**C**N**C**C**C
         *
         *
         C
         *
         *
         C
         *
         *
         C
```

1-Propanamine, N,N-dipropyl- (9CI)
Tripropylamine (8CI)

GB (exp) : 223.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 230.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 222.8+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 230.60+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
A Thermodynamic Analysis of Solvation Effects on the Basicities of Alkylamines. An Electrostatic Analysis of Substituent Effects,
J. Am. Chem. Soc. 98, 318 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C9H21N	CAS REGN : 2085-66-7

```
   C     C
   *     *
   *     *
C**C**N**C**C**C
   *     *
   *     *
   C     C
```

Propylamine, N-tert-butyl-1,1-dimethyl- (8CI)

GB (exp) : 221.9+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 230.1+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C10H8	CAS REGN : 275-51-4

```
          C.....C
          .     .
          .     .
    C.....C     C
   .        *   .
  .          * .
C            C
.            .
.            .
C            C
 .          .
  .        .
   .      .
    .    .
     .  .
      C.
```

Azulene (8CI9CI)

GB (exp) : 215.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 223.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C10H9F3	CAS REGN : 55186-75-9

```
          C
         . .
        .   .
   F  C     C**C**C
   *  .     .  +
   *  .     .  +
F**C**C     C  C
   *   .   .
   *    . .
   F     C
```

Benzene, 1-(1-methylethenyl)-4-(trifluoromethyl)- (9CI)

GB (exp) : 189.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 197.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C10H10Fe	CAS REGN : 102-54-5

```
C+++C            C+++C
*    *          *    *
*     *        *     *
*      C**Fe**C      *
*     *        *     *
*    *          *    *
C+++C            C+++C
```

Ferrocene (8CI9CI)

PA (exp) : 208+/-4 kcal/mol	Temperature : 300 K

Foster, M. S., and Beauchamp, J. L.,
Ion-Molecule Reactions and Gas-Phase Basicity
of Ferrocene,
J. Am. Chem. Soc. 97, 4814 (1975).

Method used : ICR
Bracketing relative to CH3N=NCH3 and CH3NH2.

C10H12	CAS REGN : 1195-32-0

```
          C
         . .
        .   .
      C     C**C
      .     .
      .     .
C**C**C     C
   +   .   .
   +    . .
   C     C
```

Benzene, 1-methyl-4-(1-methylethenyl)- (9CI)
Styrene, p,.alpha.-dimethyl- (8CI)

GB (exp) : 200.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 208.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C10H12N4O4	CAS REGN : 550-33-4

```
                              O
                              *
                              *
          N++C                C
         *   *               *
        *    *              *
    C..C     *         O**C
   .   .     *        *   *
  .     .    *       *    *
 N       C**N*****C        *
  .     .            *    *
   .   .             *   *
    C..N               C**C
                       *   *
                       *    *
                       O     O
```

9H-Purine, 9-.beta.-D-ribofuranosyl- (8CI9CI)

PA (exp) : >222 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)3N.

C10H12O	CAS REGN : 1712-69-2

```
          C
         . .
        .   .
      C     C**O**C
      .     .
      .     .
C**C**C     C
   +   .   .
   +     . .
   C     C
```

Benzene, 1-methoxy-4-(1-methylethenyl)- (9CI)
Anisole, p-isopropenyl- (8CI)

GB (exp) : 206.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 214.6+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C10H13N	CAS REGN : 4096-21-3

```
   C
  . .
 .   .
C     C     C*****C
.     .     *     *
.     .     *     *
C     C*****N     C
 .   .        *   *
  . .          * *
   C            C
```

Pyrrolidine, 1-phenyl- (8CI9CI)

GB (exp) : 213.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 221.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C10H13N5	CAS REGN : 715-91-3

```
       C
      . .
     .   .
    N     N
    .     .
    .     .
N%%C      C         C*****C
     .   . *        *     *
      . .   *       *     *
       C     N*****C      C
       *     *      *    *
       *     *       * *
       N+++++C         C
```

9H-Purin-1-amine, 9-cyclopentyl- (9CI)
Adenine, 9-cyclopentyl- (8CI)

PA (exp) : >222.1 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)3N

C10H13N5O4	CAS REGN : 58-61-7

```
                              O
                              *
                              *
   N      N++C                C
   %     *   *              *
   %    *    *             *
   C..C      *         O**C
  .     .    *        *   *
 .       .   *       *    *
N         C**N*****C      *
 .       .            *    *
  .     .              *   *
   C..N                C**C
                       *   *
                       *    *
                       O     O
```

Adenosine (8CI9CI)

PA (exp) : >222 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)3N.

C10H14	CAS REGN : 98-06-6

```
          C
         . .
        .   .
   C  C     C
   *  .     .
   *  .     .
C**C**C     C
   *   .   .
   *    . .
   C     C
```

Benzene, (1,1-dimethylethyl)- (9CI)
Benzene, tert-butyl- (8CI)

GB (exp) : 183.2+/-2 kcal/mol	Temperature : 300 K

Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R.,
Alkyl Substituent Effects on the Stability of Protonated Benzene,
J. Am. Chem. Soc. 96, 7162 (1974).

Method used : ICR
Equilibrium; scale based on C6H5CH3(Toluene)

Continued on next page

GB (exp) : 182.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.6+/-2 kcal/mol	Temperature : 300 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on C6H6(Benzene)

C10H14	CAS REGN : 104-51-8

```
                C
               . .
              .   .
            C     C
            .     .
            .     .
C**C**C**C**C     C
              .   .
               . .
                C
```

Benzene, butyl- (8CI9CI)

GB (exp) : 183+/-2 kcal/mol	Temperature : 300 K

Hehre, W. J., McIver, R. T., Jr., Pople, J. A., and Schleyer, P. v. R., Alkyl Substituent Effects on the Stability of Protonated Benzene, J. Am. Chem. Soc. 96, 7162 (1974).

Method used : ICR
Equilibrium; scale based on C6H5CH3(Toluene)

Continued on next page

GB (exp) : 183+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.8+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 182.2+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 190.4+/-2 kcal/mol	Temperature : 300 K

Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on C6H6(Benzene)

C10H14N2O5	CAS REGN : 50-89-5

```
          O
          *
          *
          C**C            C
         *   *            *
        *    *            *
O**C**C     *         C++C
        *    *       *    *
         *   *      *      *
          O**C*****N        C%%O
                   *      %
                    *    %
                     C%%N
                     %
                     %
                     O
```

Thymidine (8CI9CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to NH3 and CH3NH2.

C10H15N	CAS REGN : 91-66-7

```
            C
           . .
          .   .
        C     C
        .     .
        .     .
C**C**N**C     C
     *   .   .
     *     . .
     C     C
     *
     *
     C
```

Benzenamine, N,N-diethyl- (9CI)
Aniline, N,N-diethyl- (8CI)

GB (exp) : 212.10+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 229.30+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities of Amines. Hydrogen Bonding in Proton-Bound Amine Dimers and Proton-Induced Cyclization of alpha,omega-Diamines,
J. Am. Chem. Soc. 95, 3504 (1973).

Method used : MS
Equilibrium; scale based on NH3
Entropy change assumed zero

C10H19N	CAS REGN : 31023-92-4

```
   C**C
  *    *
 *      *
C       *N
*    *C* *
*  *C    *
C*C      C
 *      *
  *    *
   C**C
```

1-Azabicyclo[3.3.3]undecane (9CI)

PA (exp) : 227.9+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T., Photoelectron Spectrum and Gas-Phase Basicity of Manxine. Evidence for a Planar Bridgehead Nitrogen, J. Am. Chem. Soc. 97, 4136 (1975).

Method used : ICR
Equilibrium; scale based on CH3NH2
Van't Hoff plot

C10H23N	CAS REGN : 2016-57-1
N**C**C**C**C**C**C**C**C**C**C	
1-Decanamine (9CI) Decylamine (8CI)	
GB (exp) : >209.7 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to (CH3)2NH

C10H24N2	CAS REGN : 111-18-2

```
C**N**C**C**C**C**C**C**N**C
   *                    *
   *                    *
   C                    C
```

1,6-Hexanediamine, N,N,N',N'-tetramethyl- (8CI9CI)

GB (exp) : 226.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Equilibrium; scale based on NH3

C11H13N	CAS REGN : 4363-25-1

```
          N**C
         * *  *
        *  C   *
   C..C     *   C
  .     .   C  *
 .       .   **
C         C**C
 .       .
  .     .
   C..C
```

2H-1,4-Ethanoquinoline, 3,4-dihydro- (8CI9CI)

GB (exp) : 220.5+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.3+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C11H15N	CAS REGN : 4096-20-2

```
   C            C
  * *          . .
 *   *        .   .
C     C      C     C
*     *      .     .
*     *      .     .
C     N*****C     C
 *   *        .   .
  * *          . .
   C            C
```

Piperidine, 1-phenyl- (8CI9CI)

GB (exp) : 216.1+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 223.9+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C12H11N	CAS REGN : 122-39-4

```
   C              C
  . .            . .
 .   .          .   .
C     C        C     C
.     .        .     .
.     .        .     .
C     C*****N**C     C
 .   .          .   .
  . .            . .
   C              C
```

Benzenamine, N-phenyl- (9CI)
Diphenylamine (8CI)

GB (exp) : >193.7 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines,
Anilines, and Pyridines. An Application of Some
Bronsted Acids as Reactants in Chemical Ionization
Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to NH3

C12H16N2O6	CAS REGN : 362-43-6

```
                        O
                        %
                        %
                        C%%N
                       *    %
                      *      %
C  C                N         C%%O
 * *               * *       *
  **               *   *     *
   C**O          *     C++C
   *   *       *
   *    *     *
   *     C**C
   *    *   *
   *   *    *
   O**C     *
       *    *
        *   *
         C**O
         *
         *
         C
         *
         *
         O
```

Uridine, 2',3'-O-(1-methylethylidene)- (9CI)
Uridine, 2',3'-O-isopropylidene- (8CI)

PA (exp) : 207+/-5 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to CH3NH2 and NH3.

C12H18	CAS REGN : 87-85-4

```
      C  C
      *  *
      *  *
      C..C
     .    .
    .      .
C**C        C**C
    .      .
     .    .
      C..C
      *  *
      *  *
      C  C
```

Benzene, hexamethyl- (8CI9CI)

GB (exp) : 197.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 205.0+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C12H19N	CAS REGN : 22025-87-2

```
   C      C..C
   *     .     .
   *    .       .
C**N**C          C
        .       .
         .     .
          C..C
          *
          *
      C**C**C
          *
          *
          C
```

Benzenamine, 2-(1,1-dimethylethyl)-N,N-dimethyl- (9CI)
Aniline, o-tert-butyl-N,N-dimethyl- (8CI)

GB (exp) : 218+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 225.8+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C12H27N	CAS REGN : 102-82-9

```
C**C**C**C**N**C**C**C**C
          *
          *
          C
          *
          *
          C
          *
          *
          C
          *
          *
          C
```

1-Butanamine, N,N-dibutyl- (9CI)
Tributylamine (8CI)

GB (exp) : 224.1+/-2 kcal/mol	Temperature : 298 K
PA (exp) : 232+/-2 kcal/mol	Temperature : 298 K

Aue, D. H., Webb, H. M., and Bowers, M. T.,
Quantitative Proton Affinities, Ionization Potentials,
and Hydrogen Affinities of Alkylamines,
J. Am. Chem. Soc. 98, 311 (1976).

Method used : ICR
Calculated entropy
Equilibrium; scale based on CH3NH2

C13H10O	CAS REGN : 119-61-9

```
   C              C
  . .            . .
 .   .          .   .
C     C        C     C
.     .        .     .
.     .        .     .
C     C*****C**C     C
 .   .       +   .   .
  . .        +    . .
   C         O     C
```

Methanone, diphenyl- (9CI)
Benzophenone (8CI)

GB (exp) : ~200.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : ~208.1+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C13H13OP	CAS REGN : 2129-89-7

```
   C               C
  . .             . .
 .   .           .   .
C     C     O   C     C
.     .     +   .     .
.     .     +   .     .
C     C*****P**C     C
 .   .       *   .   .
  . .        *     . .
   C         C     C
```

Phosphine oxide, methyldiphenyl- (8CI9CI)

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N scale based
on NH3

C13H17N5O5	CAS REGN : 362-76-5

```
          C
          *
          *
          C
         ***
        * * *
       O  C  O
       *     *
       *     *
       C*****C      C+++++N
       *     *      *     *
       *     *      *     *
O**C**C      C*****N     C
        *   *        *   . .
         * *          * .   .
          O            C     C%%O
                       .     .
                       .     .
                       N     N
                         .   .
                          . .
                           C
                           %
                           %
                           N
```

Guanosine, 2',3'-O-(1-methylethylidene)- (9CI)
Guanosine, 2',3'-O-isopropylidene- (8CI)

PA (exp) : >222 kcal/mol	Temperature :

Wilson, M. S., and McCloskey, J. A.,
Chemical Ionization Mass Spectrometry of Nucleosides.
Mechanisms of Ion Formation and Estimations of
Proton Affinity,
J. Am. Chem. Soc. 97, 3436 (1975).

Method used : MS
Bracketing relative to (CH3)3N.

C13H21N	CAS REGN : 585-48-8

```
          C
         . .
        .   .
   C  C     C  C
   *  .     .  *
   *  .     .  *
C**C**C     C**C**C
   *   .   .   *
   *    . .    *
   C     N     C
```

Pyridine, 2,6-bis(1,1-dimethylethyl)- (9CI)
Pyridine, 2,6-di-tert-butyl- (8CI)

GB (exp) : 220.6+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 228.4+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C14H12	CAS REGN : 530-48-3

```
   C              C
  . .            . .
 .   .          .   .
C     C        C     C
.     .        .     .
.     .        .     .
C     C*****C**C     C
 .   .       +   .   .
  . .        +     . .
   C         C     C
```

Benzene, 1,1'-ethenylidenebis- (9CI)
Ethylene, 1,1-diphenyl- (8CI)

GB (exp) : 201.4+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 209.2+/-2 kcal/mol	Temperature : 300 K

Unpublished work by Wolf, Staley, Koppel, Taagepera, McIver, Beauchamp, and Taft.

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

C14H15OP	CAS REGN : 1733-57-9

```
   C               C
  . .             . .
 .   .           .   .
C     C     O  C     C
.     .     +  .     .
.     .     +  .     .
C     C*****P**C     C
 .   .       *   .   .
  . .        *    . .
   C         C     C
             *
             *
             C
```

Phosphine oxide, ethyldiphenyl- (8CI9CI)

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N; scale based
on NH3

C15H17OP	CAS REGN : 2959-75-3

```
   C              C
  . .            . .
 .   .          .   .
C     C     O  C     C
.     .     +  .     .
.     .     +  .     .
C     C*****P**C     C
 .   .       *   .   .
  . .        *    . .
   C         C**C  C
             *
             *
             C
```

Phosphine oxide, (1-methylethyl)diphenyl- (9CI)
Phosphine oxide, isopropyldiphenyl- (8CI)

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N; scale
based on NH3

C15H17OP	CAS REGN : 4252-88-4

```
   C       O       C
  . .      +      . .
 .   .     +     .   .
C     C***P***C     C
.     .   *   .     .
.     .   *   .     .
C     C   C   C     C
 .   .    *    .   .
  . .     *     . .
   C      C      C
          *
          *
          C
```

Phosphine oxide, diphenylpropyl

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N; scale based
on NH3

C16H19OP	CAS REGN : Not available

```
   C     O     C
  . .    +    . .
 .   .   +   .   .
C     C**P**C     C
.     .  *  .     .
.     .  *  .     .
C     C  C  C     C
 .   .   *   .   .
  . .    *    . .
   C     C     C
        **
       * *
      C  C
```

Phosphine oxide, isobutyldiphenyl-

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N; scale based
on NH3

C16H19OP	CAS REGN : 4233-13-0

```
   C       O       C
  . .      +      . .
 .   .     +     .   .
C     C***P***C     C
.     .   *   .     .
.     .   *   .     .
C     C   C   C     C
 .   .    *    .   .
  . .     *     . .
   C      C      C
          *
          *
          C**C
```

Phosphine oxide, butyldiphenyl-

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N; scale
based on NH3

C17H21OP	CAS REGN : Not available

```
   C      O      C
  . .     +     . .
 .   .    +    .   .
C     C**P**C     C
.     .  *  .     .
.     .  *  .     .
C     C  C  C     C
 .   .   *   .   .
  . .    *    . .
   C  C**C**C  C
          *
          *
          C
```

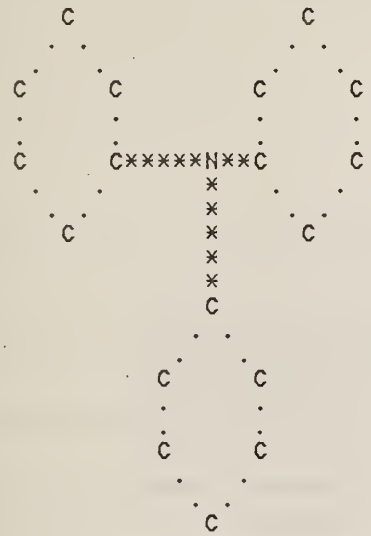
Phosphine oxide, neopentyldiphenyl-

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N scale based
on NH3

C18H15N	CAS REGN : 603-34-9



Benzenamine, N,N-diphenyl- (9CI)
Triphenylamine (8CI)

GB (exp) : >202.9 kcal/mol	Temperature : 423-473 K

Dzidic, I.,
Relative Gas-Phase Basicities of Some Amines, Anilines, and Pyridines. An Application of Some Bronsted Acids as Reactants in Chemical Ionization Mass Spectrometry,
J. Am. Chem. Soc. 94, 8333 (1972).

Method used : MS
Bracketing relative to CH3NH2

C22H31OP	CAS REGN : Not available

```
   C     O     C
  . .    +    . .
 .   .   +   .   .
C     C**P**C     C
.     .  *  .     .
.     .  *  .     .
C     C  C  C     C
 .   .   *   .   .
  . .    *    . .
   C     C     C
         *
         *
         C**C**C**C**C**C**C**C
```

Phosphine oxide, decanyldiphenyl-

PA (exp) : 220+/-3 kcal/mol	Temperature : ~400 K

Goff, S. D., Jelus, B. L., and Schweizer, E. E.
Electron Impact and Chemical Ionization Mass Spectra
of Alkyldiphenylphosphine Oxides,
Org. Mass Spectrom. 12, 33 (1977).

Method used : MS
Bracketing relative to pyridine and Me3N scale based
on NH3

Ca	CAS REGN : 7440-70-2
CA	
Calcium (8CI9CI)	
PA (exp) : >211 kcal/mol	Temperature : ~800 K

Eslava, L. A., and Porter, R. F.
A Kinetic Study of Proton Transfer Reactions of NH4+,
CH3NH3+, and PH4+ with Calcium Atoms,
Chem. Phys. Letters 52 368 (1977).

Method used : MS
Bracketing relative to NH3, PH3 and MeNH2

ClH	CAS REGN : 7647-01-0
CL	
Hydrochloric acid (8CI9CI)	
PA (exp) : 140+/-3 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).	
Method used : MS Absolute PA value estimated by assuming that for reaction RH+ + RH -> R + RH2+ the delta H ~5X TC. TC = measured translational energy of the products.	
PA (exp) : >120 kcal/mol	Temperature : 297 K
Fehsenfeld, F. C., and Ferguson, E. E. Rate Constants for the Reactions Cl+ + H2 -> HC+ + H and ClH+ + H2 -> ClH2+ + H, J. Chem. Phys. 60, 5132 (1974).	
Method used : FAG Found reaction ClH+ + H2 -> ClH2+ + H react rapidly. Since reaction Cl+ + H2 -> HCl+ + H + .22eV has a low exothermicity, they assumed HCl+ to be in ground vibrational state.	

CsHO	CAS REGN : 21351-79-1
CS*O	
Cesium hydroxide (8CI9CI)	
PA (exp) : 270.1 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA derived from delta H of reaction M+ + H2O -> (MOH2)+.	

D2	CAS REGN : 7782-39-0
H**H	
Deuterium (8CI9CI)	
PA (exp) : 98+/-4 kcal/mol	Temperature :
Harris, H. H., Crowley, M. G., Grossheim, T. R., Woessner, P. J., and Leventhal, J. J., Binding Energy of H3+, J. Chem. Phys. 59, 6181 (1973).	
Method used : MS Threshold measurement of CID of D3+ + HE->D2 + D+ + HE. Correction for collision energies distribution.	

Continued on next page

PA (exp) : 103.8+/-1.1 kcal/mol	Temperature :

Cotter, R. J., Rozett, R. W., and Koski, W. S.,
Reactions of H2O+ and D2O+ with Molecular Hydrogen.
I. Proton Affinity of Hydrogen,
J. Chem. Phys. 57, 4100 (1972).

Method used : MS
Threshold measurement of D2O+ + D2 -> D3+ + OD.
Correction for Doppler effect.

D2O	CAS REGN : 7789-20-0

O

Water-d2 (9CI)
Water, heavy (D2O) (8CI)

PA (exp) : 167+/-3 kcal/mol	Temperature :

Cotter, R. J., and Koski, W. S.,
Reaction of D3O+ with D2: Proton Affinity of Water,
J. Chem. Phys. 59, 784 (1973).

Method used : MS
Correction for Doppler effects. Deuterium affinity.
Threshold measurement of D2O+ + D2O -> D3O+ + DO.

FH	CAS REGN : 7664-39-3
F	
Hydrofluoric acid (8CI9CI)	
PA (exp) : 112+/-2 kcal/mol	Temperature : 300 K
Foster, M. S., and Beauchamp, J. L., Proton Affinity and Gas-Phase Ion Chemistry of Hydrogen Fluoroide, Inorg. Chem. 14, 1229 (1975).	
Method used : ICR Calculated entropy. Equilibrium relative to N2.	
PA (exp) : 94.3+/-1.4 kcal/mol	Temperature : 0 K
Ng, C. Y., Trevor, D. J., Tiedemann, P. W., Ceyer, S. T., Kronebusch, P. L., Mahan, B. H., and Lee, Y. T. Photoionization of Dimeric Polyatomic Molecules: Proton Affinities of H2O and HF, J. Chem. Phys. 67, 4235 (1977).	
Method used : PI AP of H2F+ from (HF)2. No temperature correction was applied in this surpersonic expansion	

FO	CAS REGN : 12061-70-0
F+O	
Oxygen fluoride	
PA (exp) : 134+/-2 kcal/mol	Temperature : 0 K
Berkowitz, J., Appelman, E. H., and Chupka, W. A. Photoionization of HOF with Mass Analysis, J. Chem. Phys. 58, 1950 (1973).	
Method used : MS Threshold measurement of reaction HOF -> HOF+	

F3N	CAS REGN : 7783-54-2

```
F**N**F
   *
   *
   F
```

Nitrogen fluoride (NF3) (8CI9CI)

PA (exp) : 151+/-10 kcal/mol	Temperature : 300 K

Holtz, D., Beauchamp, J. L., Henderson, W. G., and Taft. R. W.,
Basicity of Nitrogen Trifluoride in the Gas Phase by Ion Cyclotron Resonance,
Inorg. Chem. 10, 201 (1971).

Method used : ICR
Bracketing relative to C2H4 AND HCL.

F6S	CAS REGN : 2551-62-4

```
   F  F
   * *
   **
F**S**F
   **
   * *
   F  F
```

Sulfur fluoride (SF6), (OC-6-11)- (9CI)
Sulfur fluoride (SF6) (8CI)

PA (exp) : <144 kcal/mol	Temperature : 298 K

Gorden, R., Jr.,and Sieck, L. W.,
Ion-Molecule Reactions in Isopropanol: Implications
for its Radiolysis,
J. Res. NBS 76A, 655 (1972).

Method used : MS
Proton transfer from C2H6+ to SF6 not observed.

HI	CAS REGN : 10034-85-2
I	
Hydriodic acid (8CI9CI)	
PA (exp) : 145+/-3 kcal/mol	Temperature :

Haney, M. A., and Franklin, J. L.,
Mass Spectrometric Determination of the Proton Affinities
of Various Molecules,
J. Phys. Chem. 73, 4328 (1969).

Method used : MS
Absolute PA value estimated by assuming that
for reaction RH+ + RH -> R + RH2+; the delta H
~5X TC. TC = measured translational energy of the products.

HKO	CAS REGN : 1310-58-3
K**O	
Potassium hydroxide (8CI9CI)	
PA (exp) : 263.5 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA value derived from delta H of reaction: M+ + H2O -> (MOH2)+.	

HLiO	CAS REGN : 1310-65-2
LI*O	
Lithium hydroxide (8CI9CI)	
PA (exp) : 241.6 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA value derived from delta H of reaction M+ + H2O -> (MOH2)+	

HNaO	CAS REGN : 1310-73-2
NA*O	
Sodium hydroxide (8CI9CI)	
PA (exp) : 248.5 kcal/mol	Temperature : 300 K
Searles, S. K., Dzidic, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, J. Am. Chem. Soc. 91, 2810 (1969).	
Method used : MS PA value derived from delta H of reaction M+ + H2O = (MOH2)+	

H2	CAS REGN : 1333-74-0
H**H	
Hydrogen (8CI9CI)	
PA (exp) : 99.9+/-1 kcal/mol	Temperature :
Duben, A. J., and Lowe, J. P., Correlation Studies on H3+. I. The Wavefunctions, J. Chem. Phys. 55, 4270 (1971).	
Method used : TC SCF-MO-CI calculation.	

Continued on next page

PA (exp) : 97 kcal/mol	Temperature : 298 K

Schwartz, M. E., and Schaad, J. J.,
Ab Initio Studies of Small Molecules Using 1s
Gaussian Basis Function. II. H3+,
J. Chem. Physics 47, 5325 (1967).

Method used : TC
SCF-MO-CI calculation.

PA (exp) : 101.5 kcal/mol	Temperature :

Burt, J. A., Dunn, J. L., McEwan, M. J., Sutton, M. M.,
Rocke, A. E., and Schiff, H. I.,
Some Ion-Molecule Reactions of H3+ and the Proton
Affinity of H2,
J. Chem. Phys. 52, 6062 (1970).

Method used : FAG
Bracketing relative to O2 AND N2.

PA (exp) : 101+/-2 kcal/mol	Temperature :

Cotter, R. J., Rozett, R. W., and Koski, W. S.,
Reactions of H2O+ and D2O+ with Molecular Hydrogen.
I. Proton Affinity of Hydrogen,
J. Chem. Phys. 57, 4100 (1972).

Method used : MS
Correction for Doppler effect.
Threshold measurement of H2O+ + H2 -> H3+ + OH.

Continued on next page

PA (exp) : 96+/-4 kcal/mol	Temperature :
Harris, H. H., Crowley, M. G., Grossheim, T. R., Woessner, P. J., and Leventhal, J. J., Binding Energy of H3+, J. Chem. Phys. 59, 6181 (1973).	
Method used : MS Threshold measurement of CID of H3+ + He -> H2 + H+ +He. Correction for collision energies distribution.	

H2O	CAS REGN : 7732-18-5
O	
Water (8CI9CI)	
PA (exp) : 167+/-7 kcal/mol	Temperature : 323-373 K
Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, J. Am. Chem. Soc. 95, 2427 (1973).	
Method used : MS Bracketing relative to CH2O and C2H4	

Continued on next page

PA (exp) : 182 kcal/mol	Temperature :

Sherman, J.,
Crystal Energies of Ionic Compounds and Thermochemical Applications,
Chem. Rev. 11, 93 (1932).

Method used : CLE
Using thermochemical cycle the value of PA(H2O) was calculated from PA(NH3).

PA (exp) : 171+/-2 kcal/mol	Temperature : 296,355,426 K

Hopkins, J. M., and Bone, L. I.,
Relative Proton Affinities of Hydrogen Sulfide and Water,
J. Chem. Phys. 58, 1473 (1973).

Method used : MS
Van't Hoff plot
Equilibrium relative to H2S. Assume steady state kinetics.

PA (exp) : 165.8+/-1.8 kcal/mol	Temperature : 0 K

Ng, C. Y., Trevor, D. J., Tiedemann, P. W., Ceyer, S. T., Kronebusch, P. L., Mahan, B. H., and Lee, Y. T.
Photoionization of Dimeric Polyatomic Molecules: Proton Affinities of H2O and HF,
J. Chem. Phys. 67, 4235 (1977).

Method used : PI
AP of H3O+ from (H2O)2. No temperature correction was applied in this supersonic expansion

Continued on next page

GB (exp) : 153.3+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 169.3+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 162.3+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 170.3+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W.,
Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements,
J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

H2S	CAS REGN : 7783-06-4
S	
Hydrogen sulfide (H2S) (8CI9CI)	
GB (exp) : 165.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 173.9+/-2 kcal/mol	Temperature : 300 K
Freeman, C. G., Harland, P. W., and McEwan, M. J. The Equilibrium H3S+ + HCN = H2CN+ +H2S and the Relative Proton Affinities of HCN and H2S, Intern. J. Mass Spectrom. Ion Phys. 27, 77 (1978).	
Method used : FAG Equilibrium relative to HCN; scale based on NH3	
PA (exp) : 173.3+/-2 kcal/mol	Temperature : 296,355,426 K
Hopkins, J. M., and Bone, L. I., Relative Proton Affinities of Hydrogen Sulfide and Water, J. Chem. Phys. 58, 1473 (1973).	
Method used : MS Equilibrium relative to H2O Van't Hoff plot	

Continued on next page

PA (exp) : 177.1+/-2 kcal/mol	Temperature : 299,329,360 K
Wei, L. Y., and Bone, L. I., Ion-Molecule Reactions in Methanol and Hydrogen Sulfide, J. Phys. Chem. 78, 2527 (1974).	
Method used : MS Equilibrium; scale based on CH3OH Van't Hoff plot	
PA (exp) : 171 kcal/mol	Temperature :
Haney, M. A., and Franklin, J. L., Heats of Formation of H3O+, H3S+, and NH4+ by Electron Impact, J. Chem. Phys. 50, 2028 (1969).	
Method used : EI Appearance potential by electron impact. Correction for excess energy.	
GB (exp) : 165.9+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 173.9+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

Continued on next page

GB (exp) : 156.4+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 172.4+/-2 kcal/mol	Temperature : 600 K

Yamdagni, R., and Kebarle, P.,
Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements,
J. Am. Chem. Soc. 98, 1320 (1976).

Method used : MS
Calculated entropy
Equilibrium; scale based on NH3

GB (exp) : 172.4+/-2.5 kcal/mol	Temperature : 300 K
PA (exp) : 175.3+/-2.5 kcal/mol	Temperature : 300 K

Meot-Ner (Mautner), M., and Field, F. H.
Proton Affinities and Cluster Ion Stabilities in CO2 and CS2. Application in Martian Ionspheric Chemistry,
J. Chem. Phys. 66, 4527 (1977).

Method used : MS
Calculated entropy
The measurements done in the temperature range of 400-650k. Using the Hoff plot the H and S at 300 k were derived. Equilibrium; scale based on NH3

H2Se	CAS REGN : 7783-07-5
SE	
Hydrogen selenide (H2Se) (8CI9CI)	
GB (exp) : 166.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 174.7+/-2 kcal/mol	Temperature : 300 K
Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).	
Method used : ICR Calculated entropy Equilibrium; scale based on NH3	

H3N	CAS REGN : 7664-41-7
N	
Ammonia (8CI9CI)	
PA (exp) : >197 kcal/mol	Temperature :
Chupka, W. A., and Russell, M. E., Ion-Molecule Reactions of NH3+ by Photoionization, J. Chem. Phys. 48, 1527 (1968).	
Method used : PI NH3+ formed by photoionization and react with H2O.	
PA (exp) : 206.4 kcal/mol	Temperature :
Bleick, W. E., The Lattice Energies of the Ammonium Halides and the Proton Affinity of Ammonia, J. Chem. Phys. PA = 2, 160 (1934).	
Method used : CLE Using thermochemical cycle the PA is derived from crystal lattice energy.	

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PA (exp) : 208 kcal/mol	Temperature :

Haney, M. A., and Franklin, J. L.,
Heats of Formation of H3O+, H3S+, and NH4+ by
Electron Impact,
J. Chem. Phys. 50, 2028 (1969).

Method used : EI
Appearance potential by electron impact.
Correction for excess energy.

PA (exp) : 194+/-7 kcal/mol	Temperature :

Vetchinkin, S. I., Pshenichnov, E. A., and Sokolov, N. D.,
The Effect of the Hydrogen Bond on the Energy of the
Ionic Lattice of Ammonium Chloride and Estimation
of the Proton Affinity of an Ammonia Molecule,
Zh. Fiz. Khim. 33, 1269 (1959).

Method used : CLE
PA from crystal lattice energy, correction for hydrogen bond.

PA (exp) : 206+/-8 kcal/mol	Temperature :

Sherman, J.,
Crystal Energies of Ionic Compounds and Thermochemical
Applications,
Chem. Rev. 11, 93 (1932).

Method used : CLE
Using thermochemical cycle the PA values 209, 208.6
and 202.7 are derived from crystal lattice energy of
NH4Cl, NH4Br and NH4I respectively.

Continued on next page

GB (exp) : 185.1+/-2 kcal/mol	Temperature : 600 K
PA (exp) : 202.3+/-2 kcal/mol	Temperature : 600 K
Yamdagni, R., and Kebarle, P., Gas-Phase Basicities and Proton Affinities of Compounds between Water and Ammonia and Substituted Benzenes from a Continuous Ladder of Proton Transfer Equilibria Measurements, J. Am. Chem. Soc. 98, 1320 (1976).	
Method used : ICR Calculated entropy Equilibrium; scale based on PA(iso-C4H8)	
GB (exp) : 193.7+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 202.3+/-2 kcal/mol	Temperature : 300 K
Staley, R. H., Taagepera, M., Henderson, W. G., Koppel, I., Beauchamp, J. L., and Taft, R. W., Effects of Alkyl and Fluoroalkyl Substitution on the Heterolytic and Homolytic Bond Dissociation Energies of Protonated Amines, J. Am. Chem. Soc. 99, 326 (1977).	
Method used : ICR Calculated entropy Equilibrium.	

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PA (exp) : 205.7+/-1 kcal/mol	Temperature : 298.15 K

Meot-Ner (Mautner), M., and Field, F. H.
Proton Affinities and Cluster Ion Stabilities in CO2 and CS2. Application in Martian Ionspheric Chemistry,
J. Chem. Phys. 66, 4527 (1977).

Method used : CLE
Using thermochemical cycle the PA value is derived from crystal lattice energy. Error due to some of the thermochemical data and the similarity of crystal structure.

PA (exp) : 205.3 kcal/mol	Temperature :

Goodliffe, A. L., Jenkins, H. D. B., Martin, S. V., and Waddington, T. C.,
The Proton Affinity of Gaseous Ammonia, the Charge Distribution on the NH4+ Ion and the Lattice Energies of NH4Cl, NH4Br, and NH4I,
Mol. Phys. 21, 761 (1971).

Method used : CLE
Using thermochemical cycle the PA is derived from crystal lattice energy and the distributed charge on NH4+.

H3P	CAS REGN : 7803-51-2
P	
Phosphine (8CI9CI)	
PA (exp) : 200+/-10 kcal/mol	Temperature : 298 K
Wendlendt, W., Proton Affinity of Phosphine in the Phosphonium Halides, Science 122, 831 (1955).	
Method used : CLE Using thermochemical cycle calculate the PA value from crystal lattice energy.	
PA (exp) : 156.2+/-3 kcal/mol	Temperature :
Wada, Y., and Kiser, R. W., A Mass Spectrometric Study of Some Alkyl-Substituted Phosphines, J. Phys. Chem. 68, 2290 (1964).	
Method used : EI Appearance potential by electron impact of (CH3)3P and (C2H5)3P	

Continued on next page

PA (exp) : 194.5+/-5 kcal/mol	Temperature :

Waddington, T. C.,
Lattice Energies of Phosphonium Bromide and Iodide
and the Proton Affinity of Phosphine,
Trans. Faraday Soc. 61, 2652 (1965).

Method used : CLE
Using thermochemical cycle they calculated the PA
from crystal lattice energy and heats of formation.

PA (exp) : 186 kcal/mol	Temperature :

Haney, M. A., and Franklin, J. L.,
Mass Spectrometric Determination of the Proton Affinities
of Various Molecules,
J. Phys. Chem. 73, 4328 (1969).

Method used : MS
Delta H estimated = 5X total translational energy
of the products of RH+ + RH -> RH2+ + R.

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GB (exp) : 178.8+/-2 kcal/mol	Temperature : 300 K
PA (exp) : 187.4+/-2 kcal/mol	Temperature : 300 K

Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, R. T., Jr., Beauchamp, J. L., and Taft, R. W., Gas Phase Basicities and Relative Proton Affinities of Compounds between Water and Ammonia from Pulsed Ion Cyclotron Resonance Thermal Equilibria Measurements, J. Am. Chem. Soc. 99, 5417 (1977).

Method used : ICR
Calculated entropy
Equilibrium; scale based on NH3

H4N2	CAS REGN : 302-01-2
N**N	
Hydrazine (8CI9CI)	
PA (exp) : 221 kcal/mol	Temperature :

Jen, J. A., and Thomas, T. D., Core Ionization Potentials in Dimethyl Ether and Methyl Amine, J. Electron Spectrosc. 4, 43 (1974).

Method used : CIP
Assuming that delta H of CH4 + NH2NH3+ -> CH3NH2 + NH4+ is equal to the difference in carbon 1S ionization potentials of CH4 and CH3NH2.
CIP = core ionization potential.

H4Si	CAS REGN : 7803-62-5
SI	
Silane (8CI9CI)	
PA (exp) : 155+/-3 kcal/mol	Temperature :
Cheng, T. M. H., and Lampe, F. W., SiH5+ and the Proton Affinity of Monosilane, Chem. Phys. Letters 19, 532 (1973).	
Method used : MS Bracketing relative to C2H2 AND C3H7.	

He	CAS REGN : 7440-59-7
HE	
Helium (8CI9CI)	
PA (exp) : 41.5 kcal/mol	Temperature :
Bel'skii, V. E., and Izmailov, R. I., Proton Affinity of Atoms and Ions, Zh. Obshch. Khim. 44, 2297 (1974).	
Method used : TC Using thermochemical cycles.	

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PA (exp) : 42 kcal/mol	Temperature :
Beauchamp, J. L., Interactions between Ions and Molecules, Ed. P. Ausloos, (Plenum Press, New York and London, 1975) p. 413.	
Method used : HE Literature Survey.	

Kr	CAS REGN : 7439-90-9
KR	
Krypton (8CI9CI)	
PA (exp) : 115+/-15 kcal/mol	Temperature :
Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XVI. Effects of Additives on Ionic Reactions in Methane, J. Am. Chem. Soc. 87, 4243 (1965).	
Method used : MS Bracketing relative to H2 and CH4.	

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PA (exp) : 100.3+/-0.5 kcal/mol	Temperature :

Payzant, J. D., Schiff, H. I., and Bohme, D. K.,
Determination of the Proton Affinity from the Kinetics
of Proton Transfer Reactions. V. The Equilibrium
H3+ + Kr = KrH+ + H2 and the Relative Proton Affinity
of Kr and H2,
J. Chem. Phys. 63, 149 (1975).

Method used : FAG
Equilibrium relative to H2. Delta S estimated
from the entropies of the particles.

Mg	CAS REGN : 7439-95-4

MG

Magnesium (8CI9CI)

PA (exp) : ~198 kcal/mol	Temperature : 350 K

Po, P. L., and Porter, R. F.
High-Temperature Ion-Molecule Chemistry. A Kinetic
Study of Gas-Phase Reactions of Magnesium Atoms
with D3+, Methanium, Ammonium, and tert-C4H9+ Ions,
J. Am. Chem. Soc. 99, 4922 (1977).

Method used : MS
Bracketing relative to (CH3)2C=CH2 and NH3

Mg2	CAS REGN : 29904-79-8
Mg+Mg	
Magnesium molecule	
PA (exp) : 219+/-7 kcal/mol	Temperature : 700 K

Po, P. L., and Porter, R. F.
A Thermodynamic Study of the Reactions of Mg+(g) and MgH+(g) with Magnesium,
J. Phys. Chem. 81, 2233 (1977).

Method used : MS
Calculated entropy
From the K equilibrium of rection MgH+ + Mg(s) = Mg2H+ and using PA (Mg) = 196 and delta Hf(H+) = 365.7

NO	CAS REGN : 10102-43-9
N++O	
Nitrogen oxide (NO) (8CI9CI)	
PA (exp) : <127 kcal/mol	Temperature :

Munson, M. S. B., and Field, F. H.,
Reactions of Gaseous Ions. XVI. Effects of Additives on Ionic Reactions in Methane,
J. Am. Chem. Soc. 87, 4243 (1965).

Method used : MS
Bracketing relative to CH4.

PA (exp) : 126.9+/-1.1 kcal/mol	Temperature : 300 K

Hemsworth, R S., Payzant, J. D., Schiff, H. I., and Bohme, D. K.,
Rate Constants at 297 K for Proton Transfer Reactions with NH3 Comparisons with Classical Theories and Exothermicity,
Chem. Phys. Letters 26, 417 (1974).

Method used : FAG
Equilibrium relative to H2. Use PA (H2) from
J. Chem. Phys. 55, 4270 (1971).

N2	CAS REGN : 7727-37-9
N##N	
Nitrogen (8CI9CI)	
PA (exp) : 112.6+/-1 kcal/mol	Temperature : 298 K
Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).	
Method used : FAG Equilibrium scale based on H2. Delta S derived from theoretical entropies and entropies of iso-electronic particles.	
PA (exp) : 130+/-2 kcal/mol	Temperature :
Willis, C., Lossing, F. P., and Back, R. A. The Heat of Formation of N2H2 and the Proton Affinity of N2, Can. J. Chem. 54, 1 (1976).	
Method used : EM The PA is derived from the appearance potentials of N2+ and N2H+	

N2O	CAS REGN : 10024-97-2
O++N++N	
Nitrogen oxide (N2O) (8CI9CI)	
PA (exp) : 138.4 kcal/mol	Temperature : 298 K
Schiff, H. I., and Bohme, D. K., Flowing Afterglow Studies at York University, Int. J. Mass Spectrom. Ion Phys. 16, 167 (1975).	
Method used : FAG Calculated entropy Equilibrium; scale based on CO.	

O2	CAS REGN : 7782-44-7
O++O	
Oxygen (8CI9CI)	
PA (exp) : 100.9+/-.5 kcal/mol	Temperature : 298 K
McCulloh, K. E., To be published.	
Method used : PI Photoionization of H2O2.	

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PA (exp) : 100.4+/-1.5 kcal/mol	Temperature : 298 K

Kim, J. K., Theard, L. P., and Huntress, W. T., Jr.,
Proton Transfer Reactions from H3+ Ions to N2, O2,
and CO Molecules,
Chem. Phys. Letters 32, 610 (1975).

Method used : ICR
Equilibrium relative to H2. Entropy change estimated from the known theoretical iso-electronic counterpart entropies of the species.

PA (exp) : 100+/-1 kcal/mol	Temperature : 298 K

Fennelly, P. F., Hemsworth, R. S., Schiff, H. I.,
and Bohme, D. K.,
Determination of the Proton Affinity from the Kinetics
of Proton Transfer Reactions. IV. The Equilibrium
O2H+ + H2 = H3+ + O2 and the Relative Proton Affinity
of O2 and H2,
J. Chem. Phys. 59, 6405 (1973).

Method used : FAG
Equilibrium relative to H2. Entropy change estimated from the known theoretical iso-electronic counterpart entropies of the species.

O3S	CAS REGN : 7446-11-9
O++S++O + + O	
Sulfur trioxide (8CI9CI)	
PA (exp) : 142+/-2 kcal/mol	Temperature :
Munson, B., Smith, D., and Polley, C. The Mass Spectrum, Proton Affinity and Ion-Molecule Reactions of SO3, Intern. J. Mass Spectrom. Ion Phys. 25, 323 (1977).	
Method used : MS Bracketing relative to HBr and CO. Use delta Hf(H+) = 366.	

U	CAS REGN : 7440-61-1
U	
Uranium (8CI9CI)	
PA (exp) : 238+/-4 kcal/mol	Temperature : 400 K
Armentrout, P., Hodges, R., and Beauchamp, J. L. Metal Atoms as Superbases: the Gas Phase Proton Affinity of Uranium, J. Am. Chem. Soc. 99, 3162 (1977).	
Method used : MS Threshold measurement of UD+. Correction for D(UD+) - D(UH+) assuming delta H400 = delta H298 Entropy change assumed zero	

Xe	CAS REGN : 7440-63-3
XE	
Xenon (8CI9CI)	
PA (exp) : 118+/-11 kcal/mol	Temperature :
Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XVI. Effects of Additives on Ionic Reactions in Methane, J. Am. Chem. Soc. 87, 4243 (1965).	
Method used : MS Bracketing relative to CH4 and reaction XE+(2P1/2) + CH4.	
PA (exp) : 113.2+/-1.5 kcal/mol	Temperature : 800 K
Fehsenfeld, F. C., Lindinger, W., Schiff, H. I., Hemsworth, R. S., and Bohme, D. K. Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. VI. The Relative Proton Affinities of N2, Xe, and CO2, J. Chem. Phys. 64, 4887 (1976).	
Method used : FAG Van't Hoff plot Equilibrium relative to N2; scale based on PA (N2) = 112.6	

123.0 41
153.3 453
154.7 46
156.4 456
162.3 453
162.5 24
164.4 55
165.1 47
165.4 108,253
165.7 42,454
165.9 256,455
166.5 33
166.7 20,457
166.8 51,265
166.9 19,267
167.0 267
167.2 22
167.3 54
167.8 270
169.5 96
169.6 13
169.7 43
169.8 65
170.1 60
171.2 52,83,246
171.8 57,66
171.9 25
172.0 269
172.2 69
172.3 2,116,144
172.4 456
172.5 97
172.7 247
173.0 98
173.1 47,154,248
173.4 249-250
173.7 251
173.9 119,257
174.1 252,334
174.2 264
174.3 254
174.4 34,255
174.5 85,266
174.7 269
175.1 370
175.4 151
175.6 123
176.1 174
176.4 217
176.6 294
176.7 268
177.1 157
177.2 64
177.4 162
177.5 34
177.6 361
178.1 35

178.3 103
178.4 82
178.8 464
178.9 83
179.0 68,114
179.1 276
179.2 57,329
179.6 333
179.8 67,121
179.9 68
180.1 99,336
180.2 116
180.8 88,335
180.9 326,335,370
181.0 132
181.1 277
181.3 85,360
181.4 191
181.8 369,371,391
181.9 134,172
182.0 372-373
182.2 389,413
182.4 104,177,411
182.5 190
182.6 390-391
182.7 86
182.8 169,227
182.9 230,359,372
183.0 367,388,412-413
183.2 330,410
183.4 123
183.5 337
183.6 159
183.7 122,368
183.9 175
184.1 222
184.2 134
184.4 158
184.5 174
184.7 173,232
185.1 162,460
185.4 153
185.8 179
186.0 44
186.2 133
186.3 327
186.5 114
186.7 120
186.8 193,295
187.2 373
187.4 218
187.6 121
188.4 352-353
188.5 75
188.6 176
188.7 189
188.9 61,328

189.0 171
189.2 170
189.3 402
189.7 228
189.8 124,178,325
190.0 190,300
190.2 89
190.3 177
190.4 330
190.5 180
190.7 296
190.8 229
191.1 225,231
191.3 392
191.5 362
191.7 237
191.8 308
191.9 62,313
192.1 181
192.2 152,309
192.3 221
192.5 226
192.9 135,236
193.1 365
193.4 38,278
193.7 279,291-292,421,460
193.9 298
194.0 279,364
194.4 219
195.0 76
195.2 194,384
195.3 363
195.5 314
195.6 312
195.9 37
196.1 111
196.6 315
196.9 385
197.0 274,387
197.2 81,220
197.5 72,272
197.7 423
197.8 263
197.9 152
198.0 273
198.4 210
198.5 271
198.9 297
199.0 147,262
199.5 316
199.6 110
199.8 261
199.9 280
200.2 339,347
200.4 278
200.6 105,108,208
200.7 426

200.8 404
200.9 87,168
201.2 129,146,258
201.4 430
201.8 80
202.2 259
202.5 260
202.9 36,293,437
203.0 366,377
203.2 340-341
203.4 92,235
203.6 374
203.7 207,213
203.9 167,348
204.0 204
204.5 205
204.6 74
204.7 166
204.8 311
204.9 74
205.3 126
205.4 185
205.6 90,92,284
205.7 37
205.9 90
206.1 186,338
206.4 145,209
206.6 331
206.8 332,376,406
207.1 139
207.2 206
207.3 140
207.6 197
207.7 196
207.8 197
208.0 238
208.1 137,318
208.2 137,355
208.3 196
208.4 139
208.6 184
208.8 242
208.9 200
209.0 242
209.3 141,200,386
209.4 395
209.5 91,93
209.6 234
209.7 91,212,351,355,376,417
209.8 213
210.1 310
210.2 195
210.3 212
210.4 195
210.9 188
211.1 239
211.4 287

211.7 239
211.9 127
212.0 141
212.1 415
212.2 127,140
212.3 375
213.0 282
213.3 182,289
213.6 94,300,407
213.7 138,182
213.8 283
214.0 95
214.1 198
214.3 138,281
214.4 233
214.5 198
214.9 142,233
215.5 94
215.9 401
216.0 199,243
216.1 320,420
216.5 320
216.7 199
217.0 285
217.2 307,379
217.3 156,235
217.7 378
217.8 234
217.9 307,317
218.0 424
218.3 312
218.4 240,317
218.6 357
218.8 311
218.9 240-241
219.0 398
219.1 143
219.9 324,380
220.0 245,323
220.5 419
220.6 319,321,429
220.8 354
221.1 143
221.2 319,323
221.3 356
221.4 245
221.7 201,382
221.9 400
222.8 399
223.1 399
223.6 381
224.0 322
224.1 425
224.6 322
224.9 351
225.4 244
226.9 418

227.7	358
229.3	383

41.5 465
42.0 466
94.3 443
96.0 451
97.0 450
98.0 441
99.9 449
100.0 1,472
100.3 467
100.4 472
100.9 471
101.0 450
101.5 450
103.8 442
112.0 443
112.6 470
113.2 475
115.0 3-4,466
118.0 475
120.0 440
121.0 17
123.0 42
124.0 41
126.0 31
126.9 469
127.0 30,469
128.0 79
129.1 40
130.0 470
130.5 31
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NBS-114A (REV. 9-78)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBSIR 79-1777	2. Gov't. Accession No.	3. Recipient's Accession No.

4. TITLE AND SUBTITLE

A Compendium of Gas Phase Basicity and Proton Affinity Measurements

5. Publication Date

July 1979

6. Performing Organization Code

7. AUTHOR(S) K. N. Hartman, S. Lias, P. Ausloos, H. M. Rosenstock, S. S. Schroyer, C. Schmidt, D. Martinsen, & G. W. A. Milne

8. Performing Organ. Report No.

9. PERFORMING ORGANIZATION NAME AND ADDRESS

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, DC 20234

10. Project/Task/Work Unit No.

11. Contract/Grant No.

12. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS *(Street, City, State, ZIP)*

same as above.

13. Type of Report & Period Covered

April 1979

14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Literature values of experimental measurements, calculations and estimations of gas phase basicities and proton affinities are presented. Where appropriate they are recalculated to common values for the proton affinity of ammonia and the heat of formation of the proton. The annotated information is ordered by molecular formula following the Hill System. Indices are given to permit location of information of by numerical value of the measurement(s), the compound formula, name and synonym, and CAS Registry Number. The literature coverage is essentially complete through 1977.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

18. AVAILABILITY ☒ Unlimited

☐ For Official Distribution. Do Not Release to NTIS

☐ Order From Sup. of Doc., U.S. Government Printing Office, Washington, DC 20402, SD Stock No. SN003-003-

☒ Order From National Technical Information Service (NTIS), Springfield, VA. 22161

19. SECURITY CLASS (THIS REPORT)	21. NO. OF PRINTED PAGES
UNCLASSIFIED	562
20. SECURITY CLASS (THIS PAGE)	**22. Price**
UNCLASSIFIED	$16.25

USCOMM-DC